United States	Office of Air Quality	EPA-450/4-84-022a
Environmental Protection	Planning and Standards	October 1987
Agency	Research Triangle Park, NC 27711	

Air

♻ EPA APPENDIX E AND F TO NETWORK DESIGN AND SITE EXPOSURE CRITERIA FOR SELECTED NONCRITERIA AIR POLLUTANTS

INTRODUCTION

This report contains Appendices E and F to the previously published "Network Design and Site Exposure Criteria for Selected Noncriteria Air Pollutants," EPA-450/4-84-022 (September 1984). Appendix E contains the chemical profiles for 20 new chemicals and Appendix F contains guidance on the monitoring frequency for noncriteria air pollutants.

DISCLAIMER

Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

APPENDIX E

NETWORK DESIGN AND SITE
EXPOSURE CRITERIA FOR SELECTED
NONCRITERIA AIR POLLUTANTS

Prepared by

PEI Associates, Inc.
11499 Chester Road
Cincinnati, Ohio 45246

CONTENTS

APPENDIX E

     This appendix to the EPA report "Network Design and Site Exposure Criteria for Selected Noncriteria Air Pollutants" (EPA-450/4-84-022) dated September 1984 completes the chemical profiles begun in Appendix D; four completely new chemicals have been added. Sixteen chemicals were included in the body of the report for which no chemical profiles were included in Appendix D. Chemical profiles are included in this appendix for these chemicals and four additional pollutants: benzo(a)pyrene, 1,3-butadiene, ethylene dibromide, and 4,4'-methylenedianiline. The 20 chemicals included in this appendix are:

- benzo(a)pyrene
- 1,3-butadiene
- o-, m-, p-cresol
- p-dichlorobenzene
- dimethylnitrosamine
- ethylene dichloride
- ethylene dibromide
- ethylene oxide
- formaldehyde
- hexachlorocyclopentadiene
- maleic anhydride
- manganese
- mercury
- methylene chloride
- 4,4'-methylenedianiline
- perchloroethylene
- phenol
- phosgene
- propylene oxide
- o-, m-, p-xylene

     The information in this appendix has been reviewed by industry groups and reflects their comments.

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Chemical Name

Benzo(a)pyrene

CAS Number

50-32-8

Chemical Classification

Polynuclear aromatic hydrocarbon

Synonyms

Benzo(d,e,f)chrysene, 3,4-benzopirene, 3,4-benzopyrene,
6,7-benzopyrene, 3,4 benzpyren, benz(a)pyrene, 3,4-benzpyrene,
3,4-benz(a)pyrene, 3,4-benzypyrene, BP, B(a)P, 3,4-BP

Physical/Chemical Properties

Description:
    Yellowish crystals

Boiling Point:
    310° to 312°C (10mm)

Melting Point:
    179°C

Molecular Weight:
    252.3

Chemical Formula:
    $C_{12}H_{2C}$

Vapor Pressure:
    5.49×10^{-9} mm Hg

Vapor Density:
    Not available

Refractive Index:
    Not available

Solubility:
    Insoluble in water; slightly soluble in alcohol; soluble in
    benzene, toluene, xylene.

Log Partition Coefficient (octanol/water):
6.04

Photochemical Reactivity:
Not available

Chemical Reactivity:
Hydrogenation with platinum oxide gives 4,5-dihydrobenzo(a)
pyrene, 7, 8, 9, 10-tetrahydro(a)pyrene and perhydrobenzo(a)
pyrene. On oxidation with chromic acid or ozone, B(a)P yields
benzo(a)pyrene-1,6-quinone and benzo(a)pyrene-3,6-quineon; and
on further oxidation, benzanthrone dicarboxylic anhydride.
Electrophilic substitution occurs mainly in position 6. B(a)P
oxidizes in benzene under the influence of light and air.
When heated to decomposition, emits acrid smoke and irritating
fumes.

Environmental Fate
Very strong adsorption onto suspended solids is the dominant
transport process.
Bioaccumulation is short-term; metabolism and microbial degradation
are principal fates.

Source of Emissions

Production:
Produced in the United States by one company and distributed
by several specialty companies in quantities from 100 mg to 5
g for research purposes. Although not produced in great
quantities, it is a byproduct of combustion, and an estimated
1.8 million lb per year is released from stationary sources--96
percent from coal refuse piles, outcrops, and abandoned coal
mines; residential external combustion of bituminous coal;
coke manufacture; and residential external combustion of
anthracite coal. Has been detected in cigarette smoke at
levels ranging from 0.2 to 12.2 µg/100 cigarettes. Has been
detected in foods at levels ranging from 0.1 to 50 ppb.

Uses:
Research purposes only

Tables E-1 and E-2 present emission factors and ambient
concentrations of benzo(a)pyrene.

Storage:
In laboratory only

Transportation:
Shipped only in small (less than 5 g) quantities

TABLE E-1. EMISSION FACTORS FOR BENZO(A)PYRENE

Cigarettes	2.5 µg/100 cigarettes
Automobile exhaust	0.05-0.08 mg/liter gasoline consumed
Fuel oil combustion (large furnace)	0.13 mg/ton fuel
Fuel oil combustion (small furnace)	10.6 mg/ton fuel
Space heaters (coal)	10 mg/10^6 Btu input
Space heaters (gas)	0.2 mg/10^6 Btu input
Refuse burning	11.0 g/m³ of emitted gas
Power station (coal)	0.3 g/m³ of emitted gas
Power station (gas)	0.1 g/m³ of emitted gas
Automotive diesel	5.0 g/m³ of emitted gas
Coke oven volatiles	35.0 g/m³ of emitted gas
Water spray-tower, asphaltic concrete	<100 ng/m³
Outlet of asphalt air-blowing process	<4,000 ng/m³

Source: Verschueren, K. 1983.

TABLE E-2. BENZO(A)PYRENE CONTENT OF URBAN AIR

City	Benzo(a)pyrene, ng/m³			
	Spring	Summer	Fall	Winter
New York -Commercial	0.5-8.1	0.7-3.9	1.5-6.0	0.5-9.4
-Freeway	0.1-0.8	0.1-0.7	3.3-3.5	0.7-1.3
-Residential	0.1-0.6	0.1-0.3	0.6-0.8	0.5-0.7
Detroit -Commercial	7.2	-	-	5.0-17.0
-Freeway	-	4.0-6.0	3.4-7.3	9.2-13.7
-Residential	-	0.2	-	0.9-1.8
Atlanta	2.1-3.6	1.6-4.0	12-15	2.1-9.9
Birmingham	6.3-18	6.1-10	20-74	23-34
Cincinnati	2.0-2.1	1.3-3.9	14-18	18-26
Detroit	3.4-12	4.1-6.0	18-20	16-31
Los Angeles	0.4-0.8	0.4-1.2	1.2-13	1.1-6.6
Nashville	2.1-9.0	1.4-6.6	30-55	26
New Orleans	2.6-5.6	2.0-4.1	3.6-3.9	2.6-6.0
Philadelphia	2.5-3.4	3.5-19	7.1-12	6.4-8.8
San Francisco	0.8-0.9	0.2-1.1	3.0-7.5	1.3-2.4
Pittsburgh	-	0-23	2.9-37	8.2

Source: Verschueren K. 1983.

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Disposition:
Benzo(a)Pyrene may be disposed of in an incinerator controlled by an afterburner and an alkaline scrubber. A flammable solvent must be added.

Sampling and Analytical Methods

1. NIOSH Method 186
   a. Collection on a membrane filter.
   b. Thin layer chromatographic separation.
   c. Fluorometry.

   Detection limit:
   0.02 $\mu g/m^3$

   Possible interferences:
   This method is highly selective for B(a)P, but is sensitive to variations in technique.

2. NIOSH Method 184
   a. Collection on a filter.
   b. Extraction.
   c. Column chromatography.
   d. Spectrophotometric measurement.

   Detection limit:
   4 mg/m^3

   Possible interferences:
   Any substance that hinders the gas chromatographic separation or that absorbs radiation at the same wavelength as the sample compounds may interfere.

3. NIOSH Method 183
   a. Collection on a membrane filter.
   b. Extraction.
   c. GC separation.
   d. Spectrophotometric separation.

   Detection limit:
   0.4 mg/m^3 per 500-liter sample.

   Possible interferences:
   Any compound that has about the same GC retention time will interfere.

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4. NIOSH Method 206
   a. Sampling with glass-fiber filter.
   b. Extract ultrasonically.
   c. Enrich and measure with high pressure chromatography.

   Detection limit:
       3.3 ng/m^3

   Possible interferences:
       Any compound that is not retained in the silica column
       and absorbs light at 254 nm is measured in this procedure
       (eg. Fluorene + derivatives; polychloro-derivatives; di +
       tricyclic hydrocarbons). Most interfering compounds have
       low peak area/μg values.

Permissible Exposure Limits

	OSHA	ACGIH
TWA	Not established	Not established

OSHA indirectly limits exposure by requiring that occupational
exposure to coal tar pitch volatiles not exceed 0.2 mg/m^3 8 hr TWA.

The ACGIH lists benzo(a)pyrene as an industrial substance suspected
of carcinogenic potential for man.

Human Toxicity

Acute Toxicity:
    High acute subcutaneous toxicity in rats only.

Chronic Toxicity:
    Carcinogenesis--The activity of benzo(a)pyrene was first
    recognized decades ago, and since that time it has become a
    laboratory standard for the production of experimental tumors
    in animals that resemble human carcinomas. It ranks among the
    most potent animal carcinogens known and can produce tumors by
    single exposures to microgram quantities. It acts both at the
    site of application and at organs distant to the site of
    absorption. Its carcinogenicity has been demonstrated in
    nearly every tissue and species tested, regardless of the
    route of administration.

Mutagenicity--Benzo(a)pyrene gives positive results in nearly all
mutagenicity test systems, including the Ames Salmonella assay,
cultured Chinese hamster cells, the sister-chromated exchange test,
and the induction of DNA repair synthesis.

Teratogenicity--Limited data available.

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    CRC Press, Inc., Boca Raton, FL.

Chemical Name

1,3-Butadiene

CAS Number

106-99-0

Chemical Classification

Aliphatic hydrocarbon (unsaturated), alkadiene, olefin

Synonyms

Biethylene, biuinyl, butadieen, buta-1,3-dieen butadien,
1,3-butadien, butadiene, buta-1,3-diene, alpha-gamma-butadiene,
divinyl, crythrene, NCI-C5602, pyrrolylene, vinylethylene

Physical/Chemical Properties

Description:
Colorless gas with mild aromatic odor; easily liquified.

Boiling Point:
-4.41°C

Melting Point:
-108.9°C

Molecular weight:
54.1

Chemical Formula:
$H_2C:CHHC:CH_2$

Vapor Pressure:
17.65 psia at 0°C   1840 mm at 21°C

Vapor Density:
1.87 (air = 1)

Refractive Index:
N_D-25 = 1.4292

Solubility:
Soluble in alcohol and ether; insoluble in water.

Log Partition Coefficient (octanol/water):
1.99

Photochemical Reactivity:
    Estimated lifetime under photochemical smog conditions is less than one hour. Half-life for reaction (at 26.8°C) with HO· is 0.1 day and with O_3, 0.95 day.

Chemical Reactivity:
    Very reactive. Dangerous when exposed to heat, flame, or powerful oxidizers. Reacts violently with phenol.

Environmental Fate

The most probable environmental fate is photooxidation in the troposphere. The high vapor pressure of 1,3-butadiene precludes transport from the troposphere although it is sufficiently soluble in water to be washed out of a polluted atmosphere in rainwater. However, rapid volatilization to the atmosphere from surface water is likely. There is no information indicating 1,3-butadiene bioaccumulations.

Source of Emissions

Production:

    Ethylene coproduct (only method currently being used)
    Catalytic dehydrogenation of n-butene and n-butane (Houdry process)
    Oxidative dehydrogenation of n-butene

Uses:

    Styrene-butadiene rubber and latex
    Polybutadiene
    Adiponitrile
    Chloroprene/neoprene
    ABS rubber
    Nitrile rubber
    Numerous polymers with styrene/acrylonitrile/vinylpyridine
    Other chemicals including captan; sulfolene;tetrahydrophthalic anhydride; 1-4-hexadiene; 1-5-hexadiene; 1,4-dichlorobutene; butadiene furfural cotriemer; and R-11 pesticide

    Tables E-3 through E-8 present 1,3-butadiene production, consumption, and emission data.

Storage and Transportation:

    Although butadiene is a gas at ambient temperatures, it is stored and shipped as a pressurized liquid. It is shipped by pipeline, rail tank car, tank truck, and marine vessel. There is an extensive butadiene pipeline network between petrochemical plants on the Texas Gulf; a substantial portion of the chemical is shipped by this method. Butadiene is a flammable gas and must be handled as such. It must be isolated from any oxidizing material. Electrical equipment with spark-resistant construction must be provided.

TABLE E-3. COMPANIES PRODUCING 1,3-BUTADIENE

Company	Location	Annual capacity, 10^6 lb
Atlantic Richfield Co. ARCO Chemical Co.	Channelview, TX	450
Dow Chemical U.S.A.	Freeport, TX	85
E.I. Du Pont de Nemours & Co., Inc. Conoco Chemicals Co.	Chocolate Bayou, TX	135
El Paso Products Co.	Corpus Christi, TX	220
Exxon Chemical Americas	Baton Rouge, LA	310
	Baytown, TX	240
Mobil Chemical Co.	Beaumont, TX	80
Shell Chemical Co.	Deer Park, TX	500
	Norco, LA	500
Standard Oil Co. (Indiana) Amoco Chemicals Corp.	Chocolate Bayou, TX	180
Tenneco, Inc. Texas Petrochemical Corp.	Houston, TX	600
Texaco Chemical Co.	Port Neches, TX	500
Union Carbide Corp.	Pensulas, PR	75
	Seadrift, TX	33
	Taft, LA	75
	Texas City, TX	55
		Total 4,038

Source: PEI Associates, Inc., 1985.

TABLE E-4. USE PATTERN FOR 1,3-BD

Product	Percentage of total consumption
Styrene-butadiene rubber (SBR)	44
Polybutadiene rubber (PBR)	19
Adiponitrile	11
Styrene-butadiene copolymer latexes	8
Neoprene	7
Acrylonitrile-butadiene-styrene (ABS) resins	6
Nitrile rubber (NBR)	3
Miscellaneous (pesticides, solvents, etc.)	2
Total	100

Source: Versar, Inc., 1984.

TABLE E-5. UNCONTROLLED AND CONTROLLED VOC EMISSIONS FROM BUTADIENE
PRODUCTION BY DEHYDROGENATION OF n-BUTANE (HOUDRY PROCESS)

Source	Uncontrolled emission ratio, kg/Mg[a]	Control device or technique	Emission reduction, %	Controlled emission ratio, kg/Mg[a]
Flue gas	0.06	None	0	0.06
Reactor vent (regeneration air)	5.50	Catalytic or thermal oxidation	92	0.44
Intermittent process emissions	0.50	Elevated flare	95	0.03
Storage and handling	0.10	None[b]		0.1
Secondary	0.15	None		0.15
Fugitive	5.20	Detection and repair of major leaks plus mechanical seals	90	0.52
Total	11.51			1.30

[a] kg of VOC per Mg of butadiene produced.

[b] Pressurized storage tanks vented to the process are considered to be normal
conditions, not a separate emission control.

Source: Adapted from Standifer, 1980.

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TABLE E-6. UNCONTROLLED AND CONTROLLED VOC EMISSINS FROM BUTADIENE
PRODUCTION BY OXIDATIVE DEHYDROGENATION OF n-BUTENES

Source	Uncontrolled emission ratio, kg/Mg[a]	Control device or technique	Emission reduction, %	Controlled emission ratio, kg/Mg[a]
Flue gas	0.06	None	0	0.06
Absorption column vent	5.00	Catalytic or thermal oxidation	95	0.25
Intermittent process emissions	0.50	Elevated flare	95	0.03
Storage and handling	0.10	None[b]		0.10
Secondary	0.75	Reactor wastewater stripper-flare vented vapor	70	0.23
Fugitive	5.20	Detection and repair of major leaks plus mechanical seals	90	0.52
Total	11.61			1.19

[a] kg of VOC per Mg of butadiene produced.

[b] Pressurized storage tanks vented to the process are considered to be normal
conditions, not a separate emission control.

Source: Adapted from Standifer, 1980.

TABLE E-7. UNCONTROLLED AND CONTROLLED VOC EMISSIONS FROM BUTADIENE
PRODUCTION BY EXTRACTION FROM ETHYLENE PLANT BY-PRODUCT STREAMS

Source	Uncontrolled emission ratio, kg/Mg[a]	Control device or technique	Emission reduction, %	Controlled emission ratio, kg/Mg[a]
Flue gas	0.002	None		0.002
Hydrogenation catalyst regeneration vent	0.024	None		0.024
Methylacetylene column vent	2.100	Incineration or flare	95	0.105
Intermittent process emissions	0.250	Elevated flare	95	0.013
Storage and handling	0.100	None[b]		0.100
Secondary	0.150	None		0.150
Fugitive	2.500	Detection and repair of major leaks plus mechanical seals	90	0.250
Total	5.1			0.644

[a] kg of VOC per Mg of butadiene produced.

[b] Pressurized storage tanks vented to the process are considered to be normal conditions, not a separate emission control.

Source: Adapted from Standifer, 1980.

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TABLE E-8.   1,3-BUTADIENE MONITORING DATA

Location	Average mean value	Maximum value	Comments
Houston, TX area	5.22 2.81	88.61 33.76	incl. tunnels excl. tunnels
Los Angeles, CA	24.23	88.39	
Riverside, CA	3.98	6.19	
Atlanta, GA	5.57		
Lincoln Tunnel, NY	20.11 1.64	24.09 2.71	in tunnel outside air
Columbus, OH	0.77	5.47	
Denver, CO	1.7	7.6	only one sample set
Jones State Forest, TX*	0.67	2.41	non-urban setting

* 38 miles north of Houston, Texas.

Source: Versar, Inc., 1984.

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Disposition:
   1,3-Butadiene may be disposed of by incineration.

Sampling and Analytical Methods

1. NIOSH Method S91
    a. Adsorption on charcoal.
    b. Desorption with carbon disulfide.
    c. Gas chromatography with flame ionization detection.

    Detection limit:
        200 to 6600 mg/m^3 (91-3000 ppm) with 1-liter sample.

    Possible interferences:
        High humidity can lower vapor trapping efficiency.
        Compounds that have the same retention time at the operating parameters mentioned above may interfere.

Permissible Exposure Limits

	OSHA	ACGIH
TWA	1,000 ppm (2,200 mg/m^3)	1,000 ppm (2,200 mg/m^3)
STEL		1,250 ppm (2,750 mg/m^3)

The ACGIH has listed 1,3-Butadiene for intended changes to delete the STEL, to change the TWA to 10 ppm (22 mg/m^3) and add a notation that 1,3-Butadiene is an industrial substance suspected of carcinogenic potential for man.

Human Toxicity

Acute Toxicity:
    Vapors are irritating to eyes and mucous membranes. Inhalation of high concentrations can cause unconsciousness and death. If spilled on skin, can cause burns or frostbite (due to rapid vaporization). Human subjects tolerated 4,000 ppm for 6 hours with no apparent effects other than a slight irritation of the eyes. Tolerances to high exposures appear to develop following a single exposure. Human exposure of volunteers to 8,000 ppm for 8 hours caused eye and upper respiratory irritation.

Chronic Toxicity:
    Chronic oncology studies completed for the National Toxicology Program have indicated that 1,3-butadiene is carcinogenic in both sexes of mice and rats at levels as low as 625 ppm.

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Chemical Name

o-, m-, p-Cresol

CAS Number

95-48-7; 108-39-4; 106-44-5

Chemical Classification

Phenol

Synonyms

(2-,3-,4-,) cresol; (o-,m-,p-) cresylic acid; 1-hydroxy-(2-,3-,4-)
methylbenzene; (o-,m-,p-) hydroxytoluene; (2-,3-,4-) hydroxytoluene;
(O-,m-,p-) methylphenol; (o-,m-,p-) oxytoluene; phenol, 2-methyl-(9Cl)

Physical/Chemical Properties

Description:
    White crystals; phenol-like odor.
    Colorless to yellowish liquid; phenol-like odor.
    Crystalline mass; phenol-like odor

Boiling Point:
    191°C; 203°C; 202°C

Melting Point:
    30.9°C; 12°C; 35.3°C

Molecular Weight:
    108.1

Chemical Formula:
    $CH_3C_6H_4OH$

Vapor Pressure:
    1 mm at 38.2°C; 1 mm at 52°C; 1 mm at 53°C

Vapor Density:
    3.72; 3.72; 3.72 (air = 1.0)

Refractive Index:
    $N_D^{20} = 1.536$; $N_D^{20} = 1.544$; $N_D^{20} = 1.531$

Solubility:
    Soluble in alcohol, ether, chloroform, and hot water

Log Partition Coefficient (octanol/water):
    3.40; 2.37; 2.35

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Photochemical Reactivity:
     Reactivity toward OH· from 10 to 12 times butane. Reactivity
     toward O_3 is 10 percent of propylene. Major atmospheric
     precursor is toluene; less than 10 percent of cresols from
     toluene decay. o-Cresol reacts with oxidizing materials to
     yield quinones and benzenes; reacts in less than one day in
     air.

Chemical Reactivity:
     Reacts violently with HNO_3, oleum, and chlorosulfonic acid.
     Dangerous when heated to decomposition; emits highly toxic
     fumes. Can react vigorously with oxidizing materials.

Environmental Fate

Decomposes in a soil microflora in 1 day. An aqueous solution of
cresol is destroyed by photooxidation.

Source of Emissions

Production:
     Coal tar (from coke and gas works)
     From toluene by sulfonation or oxidation

Uses:
     Disinfectant
     Phenolic resins
     Tricresyl phosphate
     Ore flotation
     Textile scouring agent
     Organic intermediate, mfg. of salicylaldehyde
     Coumarin and herbicides
     Surfactant
     Synthetic food flavors (para isomer only)

     Tables E-9 through E-20 present data on o-, m-, p-cresol pro-
     duction, consumption, and emissions.

Storage:
     Should be stored in cool, dry, well-ventilated location, away
     from any area where the fire hazard may be acute. Should be
     protected against physical damage. Outside or detached
     storage is preferred; should be separated from oxidizing
     materials.

Transportation:
     Shipped in glass bottles, 10- and 55-gallon metal drums, 55-
     gallon metal barrels, tank trucks, tank cars, and tank barges.

Disposition:
     Cresols may be disposed of by incineration.

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TABLE E-9. CRESOLS ISOMER PRODUCERS

Company	Location	Cresol isomer capacity, 10^6 lb/yr	Cresol isomer produced, 10^6 lb/yr	Geographic coordinates, latitude/longitude
o-Cresol Producers				
Continental Oil	Newark, NJ	7.7	5.0	40 43 34/74 07 26
Fallek	Tuscaloosa, AL	9.6	6.0	33 11 00/87 34 50
Ferro	Sante Fe Springs, CA	4.5	3.0	33 56 30/118 04 18
Koppers	Oil City, PA	5.4	3.0	41 29 30/79 43 20
Merichem	Houston, TX	15.1	10.0	29 45 36/95 10 48
Stimson	Anacartes, WA	4.5	3.0	48 28 31/122 32 48
Total		46.8	30.0	
p-Cresol Producer				
Sherwin Williams	Chicago, IL	N/A[a]	21.0	41 43 04/87 36 30
m-Cresol Producers				
Koppers	Oil City, PA	N/A	0.75	41 29 30/79 43 20
Merichem	Houston, TX	N/A	0.75	29 45 36/95 10 48
Total			1.50	

[a]Not available

Source: Systems Applications, Inc., 1982.

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TABLE E-10. MIXED CRESOLS AND CRESYLIC ACID PRODUCERS

Company	Location	Tar acids capacity, 10^6 lb/yr	Cresols or cresylic acid produced, 10^6 lb/yr	Geographic coordinates, latitude/longitude
Mixed Cresol Producers				
Continental Oil	Newark, NJ	50	6	40 43 34/74 07 26
Fallek	Tuscaloosa, AL	20	2	33 11 00/87 34 50
Ferro	Sante Fe Springs, CA	30	4	33 56 30/118 04 18
Koppers	Oil City, PA	35	4	41 29 30/79 43 20
Merichem	Houston, TX	100	12	29 45 36/95 10 48
Stimson	Anacartes, WA	30	4	48 28 31/122 32 48
Total		265	32	
Cresylic Acid Producers				
Continental Oil	Newark, NJ	50	9	40 43 34/74 07 26
Crowley Tar Products	Houston, TX	30	5	29 43 50/95 14/20
Fallek	Tuscaloosa, AL	20	3	33 11 00/87 34 50
Ferro	Santa Fe Springs, CA	30	5	33 56 30/118 04 18
Koppers	Follansbee, WV	35	6	40 23 10/80 35 07
Merichem	Houston, TX	100	17	29 45 36/95 10 48
Mobile, Oil	Beaumont, TX	10	2	34 04 14/94 03 40
Stimson	Anacortes, WA	30	5	48 28 31/122 32 48
Total		305	52	

Source: Systems Applications, Inc., 1980.

TABLE E-11. 1978 END USE DISTRIBUTION OF CRESOL ISOMERS, CRESOLS, AND CRESYLIC ACID

	Isomers, Cresols, or cresylic acid used	
	10^6 lb/yr	%
o-Cresol Isomer		
2,6-ditert butyl-p-cresol (BHT)	15.0	50
Antioxidants	10.0	33
Export	5.0	17
Total	30.0	100
p-Cresol Isomer		
Phenolic resins	5.5	26
Pesticides	5.0	24
Export	10.5	50
Total	21.0	100
m-Cresol Isomer		
Pyrethroid pesticides	1.5	100
Mixed Cresols/Cresylic Acids Combined		
Tricresyl phosphate (TCP) Cresyl diphenol phosphate (CDF)}	31.0	32
Phenolic resins	20.0	21
Wire enamel solvent	20.0	21
Pesticides	8.0	8
Disinfectants/cleaning compound	3.0	3
Ore flotation	3.0	3
Miscellaneous other	7.0	7
Export	5.0	5
Total	97.0	100

Source: Systems Applications, Inc., 1980.

TABLE E-12. IDENTIFIED SOURCE LOCATIONS OF CRESOLS END-USERS

Company	Location	Production capacity, million lb/yr	Cresol usage, million lb/yr	Geographic coordinates, latitude/longitude
2,6 di-tert-buty-p-cresol (BHT) Products		o-cresol Isomer		
Ashland	Fords, NJ	12	5	40 31 20/74 20 50
Koppers	Oil City, PA	9	4	41 29 30/79 43 20
Shell	Martinez, CA	10	4	38 00 05/122 05 40
Uniroyal	Geismar, LA	5	2	30 13 30/91 00 15
Total		36	15	
Pyrethroid Pesticide Producers		m-cresol Isomer		
CPC International	Lyndhurst, NJ	NA[a]	0.5	40 47 30/74 04 34
FMC	Baltimore, MD	NA	0.5	39 14 50/76 35 30
Vertac	West Helena, AR	NA	0.5	34 36 10/90 33 45
Total			1.5	
Tricresyl Phosphate/Cresol Diphenolphosphate Producers		Mixed cresols/ cresylic Acid		
FMC	Nitro, WV	60	20	38 25 33/81 50 05
Stauffer	Gallipolis Ferry, WV	50	11	38 46 40/82 10 54
Total		110	31	

[a]Not available.

Source: Systems Applications, Inc., 1982.

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TABLE E-13. 1978 NATIONWIDE o-, m-, p-CRESOL EMISSIONS

Source	Nationwide emissions lb/yr		
	o-cresol	m-cresol	p-cresol
o-m-p-Cresol production	75,000	3,750	105,000
Mixed cresol production	24,800	34,400	20,800
Cresylic acid production	3,525	39,950	41,125
Phenolic resins production (isomer)	0	0	27,500
BHT production	15,000	0	0
Pyrethroid pesticide	0	750	0
Antioxidants production	10,000	0	0
Pesticides production	0	0	2,500
Tricresyl phosphate production	2,120	5,800	4,900
Phenolic resins	13,700	37,400	31,600
Wire enamel solvent	2,740,000	7,480,000	6,320,000
Pesticides	550	2,185	1,265
Disinfectants/cleaning compounds	411,000	1,122,000	948,000
Ore flotation agent	411,000	1,122,000	948,000
Miscellaneous, other	1,000	2,600	2,200
Coke ovens	796,080	1,104,240	667,680
Total	4,503,775	10,995,075	9,120,570

Source: Systems Applications, Inc., 1982.

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TABLE E-14. CRESOLS PRODUCTION AND END-USE EMISSION FACTORS

Source	lb lost per lb produced (used)				Deriva-tion[a]
	Process	Storage	Fugitive	Total	
Mixed cresol production	0.00190	0.00020	0.00040	0.00250	B
Cresylic acid production	0.00190	0.00020	0.00040	0.00250	B
p-Cresol production	0.0039	0.00030	0.00080	0.00500	D
BHT/antioxidants	0.0008	0.0001	0.0001	0.001	D
Phenolic resins	0.00400	0.0005	0.0005	0.00500	D
Pesticides	0.00040	0.00005	0.00005	0.00050	C
Pyrethroid pesticides	0.00040	0.00005	0.00005	0.00050	D
TCP production	0.00035	0.00005	0.00010	0.0005	C
Miscellaneous, other				0.001[b]	

[a]Basis: A - site visit data, B - state files, C - published data, D - Hydroscience estimate

[b]Based on a weighted average all of cresol uses.

Source: Systems Applications, Inc., 1982

TABLE E-15. CRESOL ISOMER EMISSIONS FROM CRESOL, ISOMER PRODUCERS

Company	Location	Emissions lb/yr			Total cresol emissions	
		Process	Storage	Fugitive	lb/yr	g/sec
o-Cresols Producers						
Continental Oil	Newark, NJ	9,500	1,000	2,000	12,500	0.18
Fallek	Tuscaloosa, AL	11,400	1,200	2,400	15,000	0.22
Ferro	Santa Fe Springs, CA	5,700	600	1,200	7,500	0.11
Koppers	Oil City, PA	5,700	600	1,200	7,500	0.11
Merichem	Houston, TX	19,000	2,000	4,000	25,000	0.36
Stimson	Anacortes, WA	5,700	600	1,200	7,500	0.11
Total		57,000	6,000	12,000	75,000	
p-Cresol Producer						
Sherwin Williams	Chicago, IL	81,900	6,300	16,800	105,000	1.51
m-Cresol Producers						
Koppers	Oil City, PA	1,425	150	300	1,875	0.03
Merichem	Houston, TX	1,425	150	300	1,875	0.03
Total		2,850	300	600	3,750	

Source: Systems Applications, Inc., 1982.

TABLE E-16. CRESOL EMISSIONS FROM MIXED, CRESOL, CRESYLIC ACID PRODUCERS

Company	Location	Emission lb/yr			Total cresol emissions	
		Process	Storage	Fugitive	lb/yr	g/sec
Continental Oil	Newark, NJ	11,400	1,200	2,400	15,000	0.22
Fallek	Tuscaloosa, AL	3,800	400	800	5,000	0.07
Ferro	Santa Fe Springs, CA	7,600	800	1,600	10,000	0.14
Koppers	Oil City, PA	7,600	800	1,600	10,000	0.14
Merichem	Houston, TX	22,800	2,400	4,800	30,000	0.43
Stimson	Anacortes, WA	7,600	800	1,600	10,000	0.14
Total		60,800	6,400	12,800	80,000	

Cresylic Acid Producers

Company	Location	Emission lb/yr			Total cresol emissions	
		Process	Storage	Fugitive	lb/yr	g/sec
Continental Oil	Newark, NJ	17,100	1,800	3,600	22,500	0.32
Fallek	Tuscaloosa, AL	5,700	600	1,200	7,500	0.11
Ferro	Santa Fe Springs, CA	9,500	1,000	2,000	12,500	0.18
Koppers	Follansbee, WV	11,400	1,200	2,400	15,000	0.22
Merichem	Houston, TX	32,300	3,400	6,800	42,500	0.61
Mobil Oil	Beachmont, TX	3,800	400	800	5,000	0.07
Stimson Lumber	Anacortes, WA	9,500	1,000	2,000	12,500	0.18
Total		89,300	9,400	18,800	117,500	

Source: System Applications, Inc., 1982.

TABLE E-17. CRESOL EMISSIONS FROM CRESOL USERS

Company	Location	Emissions lb/yr			Total cresol emissions	
		Process	Storage	Fugitive	lb/yr	g/sec
o-Cresols Producers						
2-6-Di-tert-butyl-p-cresol (BHT) producers						
Ashland	Fords, NJ	4,000	500	500	5,000	0.07
Koppers	Oil City, PA	3,200	400	400	4,000	0.06
Shell	Martinez, CA	3,200	400	400	4,000	0.06
Uniroyal	Geismar, LA	1,600	200	200	2,000	0.03
Total		12,000	1,500	1,500	15,000	
m-Cresol Producer						
Pyrethroid Pesticide Producers						
CPC International	Lyndhurst, NJ	200	25	25	250	0.004
FMC	Baltimore, MD	200	25	25	250	0.004
Vertac	West Helena, AR	200	25	25	250	0.004
Total		600	75	75	750	
Mixed Cresols/Cresylic Acid						
Tricresyl phosphate/cresyl diphenylphosphate producers						
FMC	Nitro, WV	7,000	1,000	2,000	10,000	0.14
Stauffer	Gallipolis Ferry, WV	3,850	550	1,100	5,500	0.08
Total		10,850	1,550	3,100	15,500	

Source: Systems Applications, Inc., 1982

TABLE E-18. CRESOL ISOMER EMISSIONS FROM COKE OVEN OPERATION[a]

Region	Number of sites	o-Cresol emissions lb/yr	m-Cresol emissions lb/yr	p-Cresol emissions lb/yr	Total cresol emissions lb/yr
New England	0	0	0	0	0
Middle Atlantic	15	195,750	271,500	164,175	631,425
East North Central	25	326,250	452,500	273,625	1,052,375
West North Central	3	39,150	54,300	32,835	126,285
South Atlantic	4	52,200	72,400	43,780	168,380
East South Central	9	117,450	162,900	98,505	378,855
West South Central	2	26,100	36,200	21,890	84,190
Mountain	2	26,100	36,200	21,890	84,190
Pacific	1	13,050	18,100	10,945	42,095
Total	61	796,050	1,104,100	667,645	2,567,795

[a]Basis: 107 billion lb coke produced; 0.000024 lb cresols emitted/lb coke produced; cresol composition - 25 percent p-cresol, 31 percent o-cresol, and 43 percent m-cresol in mixed cresols emitted.

Source: Systems Applications, Inc., 1982.

TABLE E-19. CRESOL ISOMER EMISSIONS FROM MIXED CRESOLS/CRESYLIC
ACID USED AS WIRE ENAMEL SOLVENT

Region	Number of sites	o-Cresol emissions lb/yr	p-Cresol emissions lb/yr	m-Cresol emissions lb/yr
New England	46	79,975	184,465	218,325
Middle Atlantic	339	589,380	1,359,440	1,608,960
East North Central	370	643,275	1,483,755	1,756,090
West North Central	84	146,040	336,855	398,680
South Atlantic	174	302,510	697,765	825,835
East South Central	44	76,500	176,445	208,830
West South Central	87	151,255	348,885	412,920
Mountain	258	448,555	1,034,620	1,224,520
Pacific	174	302,510	697,765	825,840
Total	1,576	2,740,000	6,319,995	7,480,000

Source: Systems Applications, Inc., 1982.

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TABLE E-20. CRESOL ISOMER EMISSIONS FROM MIXED CRESOLS/CRESYLIC
ACID USED AS AN ORE FLOTATION AGENT

Region	Number of sites	o-Cresol emissions lb/yr	p-Cresol emissions lb/yr	m-Cresol emissions lb/yr
New England	6	4,382	11,957	10,103
Middle Atlantic	38	27,750	75,729	63,987
East North Central	85	62,075	169,392	143,128
West North Central	145	105,890	288,964	244,159
South Atlantic	62	45,275	123,557	104,399
East South Central	40	29,211	79,714	67,354
West South Central	21	15,336	41,850	35,361
Mountain	144	105,161	286,971	242,475
Pacific	22	16,066	43,843	37,045
Total	563	411,000	1,122,000	984,000

Source: Systems Applications, Inc., 1982.

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Sampling and Analytical Methods

1. NIOSH Method 2001
    a. Absorption on silica gel.
    b. Desorption with acetone.
    c. Gas chromatography.

Detection limit:
5 to 60 mg/m^3 in a 20-liter sample

Possible interferences:
High humidity can cause lower vapor trapping efficiency.
Compounds with the same retention time may cause interference.

Permissible Exposure Limits

	OSHA (skin)	ACGIH (skin)	NIOSH (skin)
TWA	5 ppm (22 mg/m^3)	5 ppm (22 mg/m^3)	2.3 ppm (10 mg/m^3)
Odor perception	0.022 mg/m^3		

Human Toxicity

Acute Toxicity:
Cresol vapors or liquids are readily absorbed through the skin or any mucous membrane, which may cause acute and chronic poisoning. Skin contact with concentrated solutions can result in severe burns. Cresols are not sufficiently volatile to constitute a respiratory hazard under normal conditions. Systematic poisoning has rarely been reported, but it is possible that adsorption may result in damage to the kidneys, liver, and nervous systems.

Chronic Toxicity:
No reports of epidemiologic studies of worker exposures to cresol were found. No investigations of the mutagenic or teratogenic potential of cresol were found. The cresol isomers promoted DMBA-induced papillomas in mice, but no carcinomas were produced.

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Chemical Name

p-Dichlorobenzene

CAS Number

106-46-7

Chemical Classification

Chlorinated aromatic hydrocarbon.

Synonyms

P-chlorophenyl chloride; P-dichlorobenzeen; 1,4-dichloorbenzeen; P-dichlorbenzol; 1,4-dichlorbenzol; Di-chloricide; P-dichlorobenzene; 1,4-dichlorobenzene; p-dichlorobenzol; dichlorobenzene, para, solid; 1,4-dichlorobenzene; p-dichlorobenzene; evola; NCL-C54955; paracide; paracrystals; paradi; paradichlorobenzene; paradichlorobenzol; paradon; paramoth; paranuggets; parazene; PDB; PDCB; persia-perazol; santochlor.

Physical/Chemical Properties

Description:
White crystals; volatile (sublimes readily); penetrating odor.

Boiling Point:
173.7°C

Melting Point:
53°C

Molecular weight:
147.0

Chemical Formula:
$C_6H_4Cl_2$

Vapor Pressure:
10 mm at 54.8°C

Vapor Density:
5.08 (air = 1)

Refractive Index:
$N_D^{20} = 1.5285$

Solubility:
Soluble in alcohol, benzene, and ether. Insoluble in water.

Log Partition Coefficient (octanol/water):
 3.39

Photochemical Reactivity:
 Reactivity toward HO· is 50 percent of butane. Reactivity toward O_3 is 5 percent of propylene. No major atmospheric precursors.

Chemical Reactivity:
 Can react vigorously with oxidizing materials. When heated to decomposition or on contact with acid or acid fumes, will evolve toxic chloride fumes.

Environmental Fate
 Volatilizes at a relatively rapid rate; half-life less than 12 hours. Bioaccumulates more than chlorobenzene; too resistant to biodegradation to compete with volatilization. Oxidized by hydroxy radicals in atmosphere.

Source of Emissions

Production/processing:
 Chlorination of monochlorobenzene

Uses:
 Moth repellant
 General insecticide
 Germicide
 Space odorant
 Manufacture of 2,5-dichloroaniline
 Dyes
 Intermediates
 Pharmaceuticals
 Agriculture (fumigating soil)

 Tables E-21 through E-25 and Figure E-1 present p-dichlorobenzene production, consumption, and emission data.

Storage:
 Should be protected against physical damage and stored in cool, dry, well-ventilated place, away from any area where the fire hazard may be acute (outside or detached storage is preferred), separate from oxidizing materials.

Transportation:
 Should be shipped in 5-, 10-, 55-, and 110-gallon drums or tank cars.

Disposition:
 P-dichlorobenzene may be disposed of by incineration, preferably after mixing with another combustible fuel. Care must be exercised to assure complete consumption to prevent the formation of phosgene. An acid scrubber is necessary to remove the halo acids produced.

TABLE E-21. p-DICHLOROBENZENE PRODUCERS

Source	Location	1978 Estimated production,[a] 10^6 lb/yr	1978 Estimated capacity, 10^6 lb/yr	Geographic coordinates latitude/longitude
Dow	Midland, MI	9	30	43 35 28/84 13 08
Monsanto	Sauget, IL	4	12	38 35 31/90 10 11
PPG	New Martinsville, WV	13	40	39 47 22/80 51 27
Standard Chlorine	Delaware City, DE	24	75	33 33 54/75 38 47
Specialty Organics[b]	Irwindale, CA	1	2	34 06 30/117 55 48
Montrose	Henderson, NV	2	7	36 03 32/114 58 34
ICC	Niagara Falls, NY	2	8	43 03 33/79 00 55
Total		55	174	

[a]Total production was distributed per site based on capacity.
[b]Processes dichlorobenzenes from Montrose.

Source: Systems Applications, Inc. 1980.

TABLE E-22. p-DICHLOROBENZENE END-USE DISTRIBUTION 1978

End-Use	Volume, million lb/yr	Usage, %
Space deodorant	27.5	50
Moth control	22	40
Pesticide intermediate	5.5	10
TOTAL	55	100

Source: Systems Applications, Inc., 1980.

TABLE E-23. 1978 NATIONWIDE EMISSIONS OF p-DICHLOROBENZENE

Source	Nationwide emissions, lb/year
Production	398,200
Space deodorant	27,500,000
Moth control	22,000,000
Pesticide intermediate	2,750
TOTAL	49,900,950

Source: Systems Applications, Inc., 1980.

TABLE E-24. P-DICHLOROBENZENE EMISSIONS FROM PRODUCTION SITES

Source	Location	Emissions, lb/yr			Total emissions	
		Process	Storage	Fugitive	lb/year	g/s
Dow	Midland, MI	52,290	3,690	9,180	65,160	0.94
Monsanto	Sauget, IL	23,240	1,640	4,080	28,960	0.42
PPG	New Martinsville, WV	75,530	5,330	13,260	94,120	1.35
Standard Chlorine	Delaware City, DE	139,440	9,840	24,480	173,760	2.50
Specialty Organics	Irwindale, CA	5,810	410	1,020	7,240	0.10
Montrose	Henderson, NV	11,620	820	2,040	14,480	0.21
ICC	Niagara Falls, NY	11,620	820	2,040	14,480	0.21
Total		319,550	22,550	56,100	398,200	

Source: Systems Applications, Inc. 1980.

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TABLE E-25. EMISSIONS AND METEROLOGICAL STATIONS OF SPECIFIC POINT SOURCES OF p-DICHLOROBENZENE

| Company	Site	Latitude/longitude	Star station	Emissions, gm/s		
				Process	Storage	Fugitive
Dow	Midland, MI	43 35 28/084 13 08	14845	0.752976	0.053136	0.132192
Monsanto	Sauget, IL	38 35 31/090 10 11	13994	0.334656	0.023616	0.058752
PPG	New Martinsville, WV	39 47 22/080 51 27	13736	1.087632	0.076752	0.190944
Standard Chlorine	Delaware City, DE	39 33 54/075 38 47	94741	2.007936	0.141696	0.352512
Specialty Organics	Irwindale, CA	36 06 30/117 55 48	23215	0.083664	0.005904	0.014688
Montrose	Henderson, NV	36 03 32/114 58 34	23112	0.167328	0.011808	0.029376
ICC	Niagara Falls, NY	43 03 33/079 00 55	14747	0.167328	0.011828	0.029376

Source: Systems Applications, Inc. 1982.
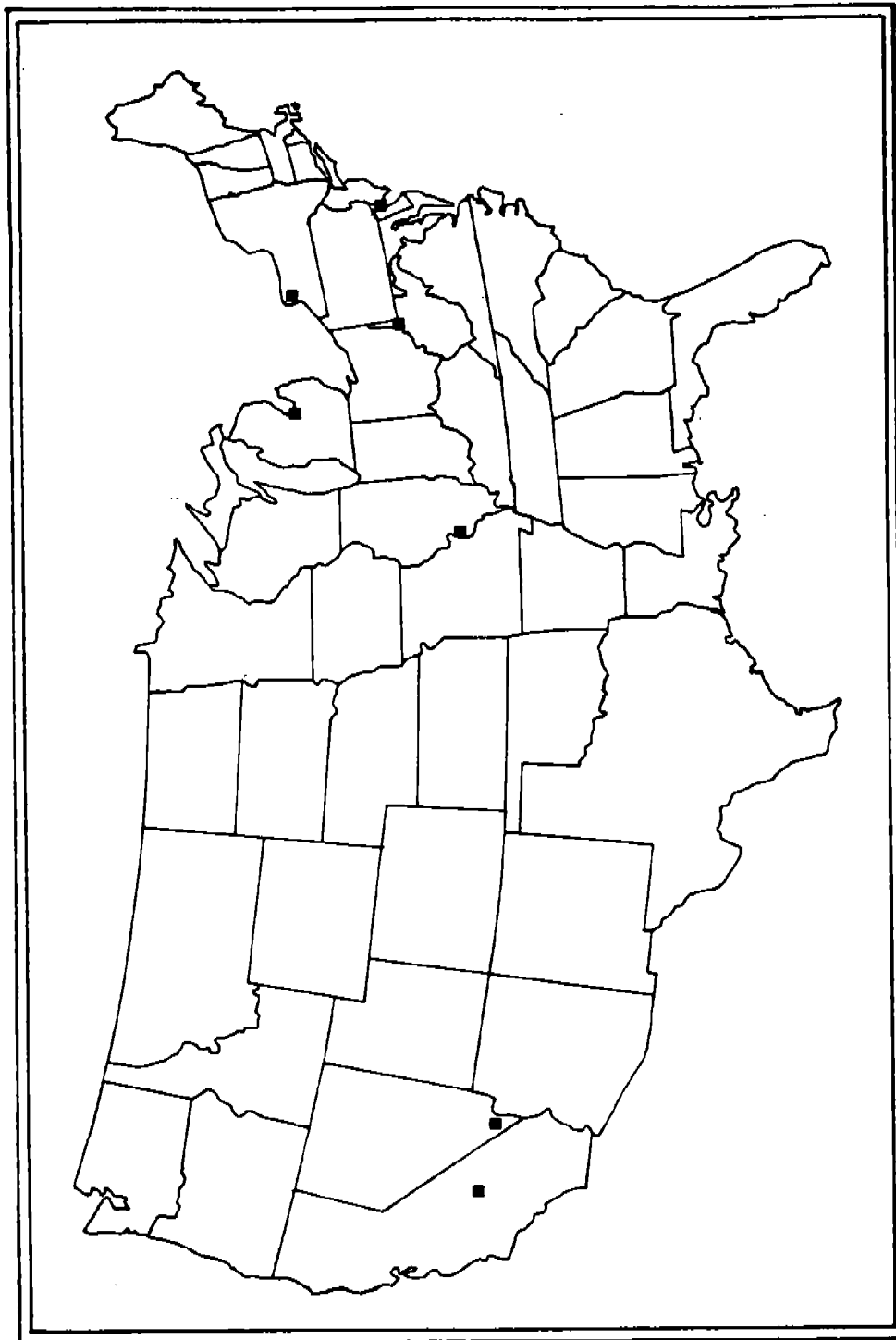
Figure E-1. Specific point sources of p-Dichlorobenzene emissions.

Source: Systems Applications, Inc. 1980

Sampling and Analytical Methods

1. NIOSH Method S281
   a. Adsorption on charcoal.
   b. Desorption with carbon disulfide.
   c. Gas chromatography.

   Detection limit:
   75 to 1350 mg/m³ (17.5-300 ppm); 170-liter sample.

   Possible interferences:
   None identified.

2. Method B (Appendix A): C_2-C_{18} hydrocarbons and other nonpolar organics with a boiling point of 100° to 175°C
   a. Whole air collection in canister.
   b. Cryogenic concentration.
   c. Gas chromatography/flame ionization detection.

   Detection limit:
   0.1 ppb per 100-ml sample.

   Possible interferences:
   Storage times greater than a week are not recommended.

3. Method C (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with a boiling point between 60° and 200°C
   a. Adsorption on Tenax (resin adsorption/solvent desorption may be used).
   b. Thermal desorption.
   c. Gas chromatography/mass spectrometry analysis (gas chromatography/electron capture detection or photoionization detection may also be used).

   Detection limit:
   1 to 200 ppt per 20-liter sample.

   Possible interferences:
   Blank levels usually limit sensitivity artifacts due to reactive components (O_3, NO_x). Sample can be analyzed only once.

4. Method D (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with a boiling point of 60° to 200°C
   a. Adsorption on Tenax (resin adsorption/solvent desorption may be used).
   b. Thermal desorption into canisters.
   c. Gas chromatography/flame ionization detection or gas chromatography/mass spectrometry analysis. (Gas chromatography/electron capture detection or photoionization detection also may be used.)

Detection limit:
0.01 to 1 ppb per 20-liter sample.

Possible interferences:
Blanks and artifact problems, as in Method C.

Permissible Exposure Limits

	OSHA	ACGIH
TWA	75 ppm (450 mg/m^3)	75 ppm (450 mg/m^3)
STEL		110 ppm (675 mg/m^3)

Human Toxicity

Acute Toxocity:
Toxicity is high orally; moderate via intraperitoneal or inhalation. Has been reported to cause liver injury in humans.

Chronic Toxicity:
Carcinogenic determination in both animals and humans is indefinite. Currently tested by the National Toxicology Program for carcinogenesis bioassay as of January 1983.

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Chemical Name

Dimethylnitrosamine

CAS Number

62-75-9

Chemical Classification

Nitrosamine

Synonyms

Dimethylnitrosamin; dimethylnitrosamine; N,N-dimethyl-nitrosamine; dimethylnitrosoamine; DMN; DMNA; N_1-methyl-N-nitrosomethanamine; NDMA; nitrosodimethylamine; N-nitrosodimethylamine.

Physical/Chemical Properties

Description:
Yellow liquid

Boiling Point:
152°C

Melting Point:
Not available

Molecular Weight:
74.1

Chemical Formula:
$(CH_3)_2N_2O$

Vapor Pressure:
Not available

Vapor Density:
2.56 (air = 1)

Refractive Index:
$N_D^{20} = 1.4358$

Solubility:
Soluble in water, alcohol and ether.

Log Partition Coefficient (octanol/water):
Not available

Photochemical Reactivity:
Photochemically reactive

45

Chemical Reactivity:
Strong oxidants (peracids) oxidize it to the corresponding
nitrosamine; can be reduced to the corresponding hydrazine
and/or amine. Relatively resistant to hydrolysis but can be
easily split by hydrogen bromide in acetic acid. When heated,
it dampens to emit NO_x.

Environmental Fate
Biodegradation of 0.01 mg/liter is 100 percent in 15 days in both
freshwater and seawater.

Source of Emissions

Production/processing:
From sodium nitrile and dimethyl amine hyperchloride.

Uses:
Prior to April 1, 1976, NDMA was used in the United States as
an intermediate in the production of 1,1-dimethyl hydrazine, a
storable liquid rocket fuel. No evidence of present use
except for research purposes.

Storage:
Mixture containing 1 percent or more NDMA must be maintained
in isolated or closed systems. Entrance to regulated area
posted "Cancer-Suspect Agent Exposed in This Area. Impervious
Suit Including Gloves, Boots, and Air-Supplied Hood Required
at All Times. Authorized Personnel Only."

Transportation:
Certain procedures must be followed in movement of material
and in case of accidental spills and emergencies. OSHA
Standards, Subpart Z, Section 1910.1016.

Disposition:
Dimethyl nitrosamine may be disposed of by pouring over soda
ash, neutralizing with HCl.

Sampling and Analytical Methods

1. NIOSH Method 252
    a. Tenax GC absorption.
    b. Thermal desorption with the purge.
    c. Capillary gas-liquid chromatography.
    d. Mass spectrometry.

    Detection limit:
    0.5 ppt to 10 ppb per 150-liter sample.

Possible interferences:
Materials having background ions of m/e 74 ($C_2H_8N_3$, $C_2H_4NO_2$, $C_6H_6N_2O$, C_3H_3Cl, C_3H_6S, $C_3H_6O_2$, or $C_3H_{10}N_2$) if at the same retention time as DMN.

2. NIOSH Method 299
   a. Adsorption on Tenax-GC.
   b. Thermal adsorption.
   c. GC-NPD.

Detection limit:
2-1000 gm/m³ per 5-liter sample.

Possible interferences:
Any compound that has the same retention time as the analyte is a potential interferent. Process is most selective for nitrogen or phosphorous containing compounds.

3. Method M (Appendix A)
   a. Adsorption on Thermosorb N.
   b. Thermal desorption.
   c. Gas chromatography/mass spectrometry or thermal energy detectors (in relatively "clear" environments, a gas chromatography/nitrogen phosphorus detection approach may be used).

Detection limit:
25 mg/m³ per 200-liter sample.

Possible interferences:
Thermal energy analyzer is a nitrosamine-specific detector and is rather expensive. Gas chromatography/nitrogen phosphorus detection may be a less expensive alternative in many situations.

Permissible Exposure Limits

	OSHA	ACGIH
TWA	Not established	Not established

Specific regulations regarding use of a regulated area and labeling requirements, are presented in Section 1910.1016 of Subpart Z of the Occupational Safety and Health Standards. The ACGIH has listed dimethyl nitrosamine as an industrial substance suspected of carcinogenic potential for man (skin).

Human Toxicity

Acute Toxicity:
High oral, inhalation, intraperitoneal, and subcutaneous toxicity. Has caused fatal liver disease in humans.

Chronic Toxicity:
> There is sufficient evidence to substantiate a carcinogenic
> effect in many experimental animal species. Similarities in
> its metabolism by human and rodent tissues have been demon-
> strated. Although no epidemiological data are available,
> dimethylnitrosamine should be regarded (for practical pur-
> poses) as if it were carcinogenic to humans.

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    Company, New York.

Weast, R. T. 1981. CRC Handbook of Chemistry and Physics. 61st Edition.
    CRC Press, Inc., Boca Raton, FL.

Chemical Name

Ethylene dichloride

CAS Number

107-06-2

Chemical Classification

Chlorinated hydrocarbon (unsaturated)

Synonyms

Aethylenchlorid; 1,2-bichloroethane; bichorure d'ethylene; berer sol; brocide; chlorure d'ethylene; cloruro di ethene; destruxol borer-sol; 1,2-dichloroethaan; 1,2-dichlor-aethan; dichloremulsion; 1,2-dichlorethane; dichlor-mulsion; dichloro-1,2-ethane; alpha-beta-dichloroethane; sym-dichloroethane; 1,2-dichloroethane; di-chloroethylene; 1,2-dichloroetano; Dutch liquid; Dutch oil; EDC; Ent 1,656; ethane dichloride; ethyleendichloride; ethylene chloride; ethylene dichloride; ethylene dichloride (DOT); 1,2-ethylene dichloride; freon 150; glycol dichloride; NCI-00511.

Physical/Chemical Properties

Description:
   Colorless oily liquid; chloroform-like odor; sweet taste

Boiling Point:
   83.5°C

Melting Point:
   -35.5°C

Molecular Weight:
   100.0

Chemical Formula:
   $ClCH_2CH_2Cl$

Vapor Pressure:
   100 mm at 29.4°C

Vapor Density:
   3.35 (air = 1)

Refractive Index:
   N_D^{20} = 1.445

Solubility:
   Miscible with most common solvents; slightly soluble in water.

49

Log Partition Coefficient (octanol/water):
1.48

Photochemical Reactivity:
Evaporates rapidly from water to the atmosphere, where it is destroyed by photooxidation.

Chemical Reactivity:
Stable to water, acids, and bases, and also resists oxidation. Incompatible with dinitrogen tetroxide, metals.

Environmental Fate

Due to a high vapor pressure, volatilization to the atmosphere is rapid and is the major transport process. Photooxidation in the troposphere may be a predominant fate. Photooxidation in the aquatic environment occurs at a slow rate.

Source of Emissions

Production/processing:
Action of chlorine on ethylene with subsequent distillation, with metalic catalyst.
Reaction of acetylene and HCl.

Uses:
Vinyl chloride solvent
Lead scavenger in antiknock gasoline
Paint, varnish, and finish remover
Metal degreasing
Soaps and scouring compounds
Wetting and penetrating agents
Organic synthesis
Ore flotation

Tables E-26 through E-30 present ethylene dichloride production, consumption, and emission data.

Storage and Transportation:
Protect against physical damage. Outside or detached storage is preferable. Inside storage should be in a standard flammable-liquids storage room or cabinet, separate from oxidizing materials. Shipped by 1-gallon cans, 5- to 55-gallon metal drums, tank cars, and tank barges.

Disposition:
Ethylene dichloride may be disposed of by incineration, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent formation of phosgene. An acid scrubber is necessary to remove the halo acids produced. Alternatively, ethylene dichloride may be recovered from process off-gases.

TABLE E-26. ETHYLENE DICHLORIDE PRODUCERS AND MAJOR CONSUMERS
(January 1, 1979, production capacities in thousands of metric tons)

Producer	Location	Capacity	VCM	1,1,1-TCE	TCE	PCE	EA	VDCM	Scavenger
Borden Chemical	Geismar, LA	524	224						
Conoco Chemical	Lake Charles, LA	145	525						
Diamond Shamrock	Deer Park, TX	719	749		17	45			
Diamond Shamrock	La Porte, TX	726	150	167	51	0[b]	60	45[c]	
Dow Chemical	Freeport, TX	499	525			0[b]			
Dow Chemical	Oyster Creek, TX					0[b]			
Dow Chemical	Pittsburg, CA								
Dow Chemical	Plaquemine, LA	953	936	112				45[c]	20[c]
Du Pont	Antioch, CA				0[b]				
Du Pont	Corpus Christi, TX								20[c]
Du Pont	Deepwater, NJ								
Ethyl Corporation	Baton Rouge, LA	318	248		15	14		20[c]	20[c]
Ethyl Corporation	Houston, TX	118							
B. F. Goodrich	Calvert City, KY	454	749						15[c]
Houston Chemical	Beaumont, TX								
ICI America[a]	Baton Rouge, LA	318	224						
Monochem	Geismar, LA		0[b]						

(continued)

TABLE E-26 (continued)

Producer	Location	Capacity	VCM	1,1,1-TCE	TCE	PCE	EA	VDCM	Scavenger
Malco Chemical	Freeport, TX	544	229	130	68	54		30[c]	5[c]
PPG Industries	Lake Charles, TX	379	375						
PPG Industries	Guayanilla, PR	635	629						
Shell Chemical	Deer Park, TX	544	525						
Shell Chemical	Morco, LA	154	130						
Stauffer Chemical	Carson, CA								
Stauffer Chemical	Louisville, KY					0[b]			
Union Carbide	Taft, LA	68					70		
Union Carbide	Texas City, TX	68					60		
Vulcan Chemical	Geismar, LA	150		0[b]		41			
Vulcan Chemical	Wichita, KS					0[b]			
Total		7,316	6,218	409	151	154	190	140	80

[a]Plant was purchased from Allied Chemical in September 1978.
[b]Process does not use EDC as a feedstock
[c]Rough order estimates.

Source: SRI International, 1979.

TABLE E-27. ESTIMATED ATMOSPHERIC EMISSIONS OF ETHYLENE DICHLORIDE FOR 1977

	Emissions, 1,000 mt/yr
EDC production	
Fugitive	5.2
Storage	14.5
Direct chlorination	6.3
Oxychlorination	17.9
Subtotal	43.9
Production in using EDC as Feedstock	
VCM	1.1
1,1,1-TCE	0.4
TCE	0.2
PCE	0.3
EA	0.3
VDCM	0.2
Lead scavenger	0.2
Subtotal	2.7
Automobile Gasoline	
Service stations	0.1
Auto emissions	1.2
Subtotal	1.3
Other	
Dispersive uses	5.0
Transportation[a]	0.0
Waste disposal[a]	0.0
Total	52.9

[a]Not included. Rough order estimates place these emissions at much less than 2,400 mt/yr for transportation and much less than 29,000 mt/yr for waste disposal.

Source: SRI International, 1979.

TABLE E-28. ESTIMATED ATMOSPHERIC EMISSIONS FROM ETHYLENE DICHLORIDE PRODUCTION FACILITIES

Plant	Location	Production[a] 10³ mt/yr	Emissions, g/s				Total
			Fugitive	Storage	Direct	Oxychlorination	
Conoco	Lake Charles, LA	372	11.8	33.0	12.8	12.6	70.2
Diamond	Deer Park, TX	103	3.3	9.1	2.6	1.9	16.9
Diamond	La Porte, TX	510	16.2	45.3	17.8	15.8	95.1
Dow	Freeport, TX	515	16.3	45.7	20.5	67.3	149.8
Dow	Oyster Creek, TX	354	11.2	31.4	12.4	0.0	55.0
Dow	Plaquemine, LA	678	21.5	60.1	24.4	99.5	205.5
Ethyl	Baton Rouge, LA	226	7.2	20.1	8.3	43.7	79.3
Ethyl	Houston, TX	84	2.7	7.5	5.9	0.0	16.1
Goodrich	Calvert City, KY	322	10.2	28.6	7.5	26.6	72.9
ICI America	Baton Rouge, LA	226	7.2	20.1	10.5	70.6	108.4
PPG	Lake Charles, LA	386	12.3	34.3	20.8	0.0	67.4
PPG	Guayanilla, PR	269	8.5	23.9	9.4	41.4	83.2
Shell	Deer Park, TX	451	14.3	40.0	20.8	27.1	102.2
Shell	Morco, LA	386	12.3	34.3	13.5	59.4	119.5
Stauffer	Carson, CA	109	3.5	9.7	5.3	19.6	38.1
Union Carbide	Taft, LA	48	1.5	4.3	3.4	0.0	9.2
Union Carbide	Texas City, TX	48	1.5	4.3	3.4	0.0	9.2
Vulcan	Geismar, LA	107	3.4	9.5	0.0	80.8	93.7
Total		5,194	164.9	461.2	199.3	566.3	1,391.7

[a]Assumed to be 71 percent of production capacity.

Souce: SRI International, 1979.

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TABLE E-29. ESTIMATED EDC ATMOSPHERIC EMISSIONS FOR PLANTS THAT USE ETHYLENE DICHLORIDE AS A FEEDSTOCK (g/s)

Producer	Location	VCM	1,1,1-TCE	TCE	PCE	EA	VDCM	Lead scavenger	Total
Borden Chemical	Geismar, LA	1.2							1.2
Conoco Chemical	Lake Charles, LA	2.9							2.9
Diamond Shamrock	Deer Park, TX			0.7	1.6				2.3
Diamond Shamrock	La Porte, TX	4.1							4.1
Dow Chemical	Freeport, TX	0.8	5.6	2.0		2.7	2.3		13.4
Dow Chemical	Oyster Creek, TX	2.9							2.9
Dow Chemical	Plaquemine, LA	5.1	3.7						8.8
Du Pont	Antioch, CA						2.3	1.1	3.4
Du Pont	Deepwater, NJ							1.1	1.1
Ethyl Corporation	Baton Rouge, LA	1.4		0.6	0.5			1.1	3.6
Ethyl Corporation	Houston, TX							1.1	1.1
B. F. Goodrich	Calvert City, KY	4.1							4.1
Houston Chemical	Beaumont, TX							0.9	0.9
ICI America	Baton Rouge, LA	1.2							1.2
Malco Chemical	Freeport, TX							0.3	0.3
PPG Industries	Lake Charles, TX	1.3	4.3	2.7	1.9		1.5		11.7
PPG Industries	Guayanilla, PR	2.1							2.1

(continued)

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TABLE E-29 (continued)

Producer	Location	VCM	1,1,1-TCE	TCE	PCE	EA	VDCM	Lead scavenger	Total
Shell Chemical	Deer Park, TX	3.4							3.4
Shell Chemical	Morco, LA	2.9							2.9
Stauffer Chemical	Carson, CA	0.7							0.7
Union Carbide	Taft, LA					3.2			3.2
Union Carbide	Texas City, TX					2.7			2.7
Vulcan Chemical	Geismar, LA				1.5				1.5
Total		34.1	13.6	6.0	5.5	8.6	6.1	5.6	79.5

Source: SRI International, 1979.

Detection limit:
  0.01 to 1 ppb per 20-liter sample

Possible interferences:
  Blanks and artifact problems as in Method C.

Permissible Exposure Limits

	OSHA	ACGIH	NIOSH
TWA	50 ppm	10 ppm (40 mg/m^3)	1 ppm (4 mg/m^3)
STEL		15 ppm (60 mg/m^3)	
Ceiling	100 ppm		2 ppm (8 mg/m^3)
Peak	200 ppm (5 min in 3 h)		

The ACGIH has listed ethylene dichloride for intended changes to delete the STEL.

Human Toxicity

Acute Toxicity:
  Most injurious exposures are acute episodes occurring because of accidental or industrial exposure. Ingestion of 20 to 50 ml is often fatal within a few days. Blood disorders appear characteristic of injection, and clotting difficulties are the most common. Death most often is attributed to circulatory and respiratory failure with varying degrees of liver and kidney damage. The effect of acute exposure to DCE by skin absorption and inhalation is similar to those following ingestion, although blood disorders are less prominent. Headache, weakness, eye irritation, cyanosis, nausea, and vomiting appear first, followed by loss of consciousness and respiratory and circulatory failure. Postmortem findings often include damage to the liver, kidneys, and lungs.

Chronic Toxicity:
  In tests by the National Cancer Institute ethylene dichloride has been shown to be carcinogenic in both rats and mice and therefore should be considered as a suspected human carcinogen.

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Sampling and Analytical Methods

1. NIOSH Method 1003
   a. Charcoal absorption.
   b. Carbon disulfide desorption.
   c. Gas chromatography.
   d. Flame ionization detector.·

   Detection limit:
   0.7 ppm for ethylene dichloride per 3-liter sample
   0.6 ppm for p-dichlorobenzene per 3-liter sample

   Possible interferences:
   None identified.

2. Method B (Appendix A): C_2-C_{18} hydrocarbons and other nonpolar organics with a boiling point of 100° to 175°C.
   a. Whole air collection in canister.
   b. Cryogenic concentration.
   c. Gas chromatography/flame ionization detection (gas chromatography/electron capture detection may also be used).

   Detection limit:
   0.1 ppb per 100-ml sample

   Possible interferences:
   Storage times greater than a week are not recommended.

3. Method C (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with boiling point between 60° and 200°C.
   a. Adsorption on Tenax.
   b. Thermal desorption.
   c. Gas chromatography/mass spectrometry analysis (gas chromatography/electron capture detection also may be used).

   Detection limit:
   1 to 200 ppt per 20-liter sample

   Possible interferences:
   Blank levels usually limit sensitivity; artifacts due to reactive components (O_3, NO_x) can be a problem. Sample can be analyzed only once.

4. Method D (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with boiling point of 60° to 200°C.
   a. Adsorption on Tenax.
   b. Thermal desorption into canisters.
   c. Gas chromatography/flame ionization detection, or gas chromatography/mass spectrometry analysis (gas chromatography/electron capture detection also may be used.)

TABLE E-30. ESTIMATED 1977 EDC EMISSIONS AS SOLID WASTE
AND TO WATER FROM ETHYLENE DICHLORIDE PRODUCTION

	Solid waste	Water
Emission factor, kg/mt		
Direct chlorination	1.5	2.9
Oxychlorination	2.8	4.6
Emissions,[a] 1000 mt/yr		
Direct chlorination	4.5	8.5
Oxychlorination	6.1	10.0
Total emissions	10.6	18.5

[a]Assumes 58 percent direct chlorination and 42 percent oxychlorination and an EDC production of 5,194,000 mt/yr.

Source: SRI International, 1979.

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Chemical Name

Ethylene dibromide

CAS Number

106-93-4

Chemical Classification

Halogenated hydrocarbon (unsaturated)

Synonyms

Aethylenbromid; bromofume; bromuro di etile; celmide; DBE; 1,2-dibromaethan; 1,2-dibromoethano; dibromoethane; alpha-beta-dibromo-ethane; sym-dibromoethane; 1,2-dibromoethane; 1,2-dibromoethane (DOT); dibromure d'ethylene; 1,2-dibromethaan; dow fume 40; dowfume EBD; dowfume W-8; dowfume W-85; dwubrometan; EDB; EDB-85; E-D-Bee; ENT 15,349; ethylene bromide; ethylene dibromide; ethylene dibromide (DOT); 1,2-ethylene dibromide; fumo-gas; glycol bromide; glycol dibromide; iscobrome-D; kopfume; NCI-C00522; nephis; pestmaster; pestmaster EDB-85; soilbrom-40; soilbrom-85; soilbrome-85; soilbrom-90EC; soilfume; unifume.

Physical/Chemical Properties

Description:
     Colorless, nonflammable liquid, sweet odor, emulsifiable.

Boiling Point:
     131°C

Melting Point:
     9°C

Molecular Weight:
     187.9

Chemical Formula:
     $BrCH_2CH_2Br$

Vapor Pressure:
     17.4 mm at 30°C

Vapor Density:
     6.48 (air = 1)

Refractive Index:
     $N_D^{20} = 1.5387$

Solubility:
Miscible with most solvents and thinners; slightly soluble in water.

Log Partition Coefficient (octanol/water):
Not available

Photochemical Reactivity:
Ethylene dibromide resists atmospheric oxidation by peroxides and ozone, typically showing half-lives in excess of 100 days in those reactions. Generally less reactive in the atmosphere than corresponding alkanes or olefins.

Chemical Reactivity:
Reacts as alkylating agent and liberates bromide. The chemical has a half-life of 5 to 10 days toward hydrolysis under neutral conditions at ambient temperature in an aquatic environment. Generally inert at normal temperatures, although slight decomposition may result from exposure to light. It is hydrolized to ethylene glycol and bromothanol at elevated temperatures. When heated to 340° to 370°C, ethylene dibrodmide decomposes to vinyl bromide and hydrobromic acid. The terminal halogen atoms are reactive, which makes the compound a useful synthetic intermediate. It is the least expensive organic bromine compound available.

Environmental Fate
C-Br bond can photolyze in atmosphere. Photooxidation is probably important in the atmosphere. Volatilization is the major transport mechanism. It is not known whether rates of atmospheric degradation are sufficient to handle the environmental burden adequately. In about 2 months, EDB is converted almost completely and quantitatively to ethylene in soil culture.

Source of Emissions

Production:
Action of bromine on ethylene.

Uses:
Scavenger for lead in gasoline (over 85 percent, used for this purpose. This use will be phased out as leaded gasoline is phased out.)
Grain fumigant
General solvent
Waterproofing preparations
Organic synthesis, including vinyl bromide
Fumigant for tree crops

Tables E-31 through E-35 present ethylene dibromide production, consumption, and emission data.

TABLE E-31. CAPACITIES OF ETHYLENE DIBROMIDE MANUFACTURING AND FORMULATING FACILITIES

Location	EDB capacity, 10^6 kg	Production of vinyl bromide	Production of fumigant	TEL[a] capacity, 10^6 kg	Estimated EDB[b] use for TEL, 10^6 kg
Arkansas					
El Dorado					
Great Lakes Chemical Corp.	23		x		
Magnolia					
Dow Chemical Co	14		x		
Ethyl Corp. (Bromet Co.)	68	x	x		
Total	82				
California					
Antioch					
E. I. Du Pont de Nemours & Co., Inc.				79	14
Louisiana					
Baton Rouge					
Ethyl Corporation				79	14
Michigan					
Midland					
Dow Chemical Company	39	x	x		
New Jersey					
Deepwater					
E. I. Du Pont de Nemours & Co., Inc.				79	14
Texas					
Beaumont					
Houston Chemical Company (PPG Industries)	16		x	54	10
Freeport					
Nalco Chemical Company				18	3
Pasadena					
Ethyl Corporation				79	14

Source: SRI International, 1978.

[a] Tetraethyl lead.

[b] Ethylene dibromide.

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TABLE E-32. ESTIMATES OF ANNUAL AVERAGE ETHYLENE DIBROMIDE
CONCENTRATIONS FOR SELECTED SMSAs

SMSA	Population	Area $10^9 m^2$	Automobile registration	Emission rate 10^{-11} g/s-m^2	Wind speed m/s	EDB[b] concentration	
						10^{-3} µg/m^3	ppt
SMSAs >2,000,000							
Pittsburgh	2,333,600	7.8	2,358,600	4.8	5	2.1	0.3
San Francisco	3,135,900	6.2	688,300	1.8	3	1.4	0.2
SMSAs 1,000,000 - 2,000,000							
Columbus, OH	1,055,900	6.2	567,803	1.7	5	0.66	0.90
Milwaukee	1,423,000	3.7	642,531	2.8	5	1.2	0.2
SMSAs 500,000 - 1,000,000							
Sacramento	851,300	8.7	439,803	0.80	3	0.60	0.08
Providence - Warwick - Pawtucket	854,400	2.4	869,100	5.8	7	1.9	0.2
SMSAs 250,000 - 500,000							
Wichita	375,600	6.2	221,715	0.57	7	0.18	0.02
Harrisburg	425,500	4.1	198,997	0.77	5	0.35	0.05

[a]Assumes 80 percent of vehicles use leaded gasoline.
[b]Ethylene dibromide.

Source: SRI International, 1978.

TABLE E-33. ESTIMATES OF AVERAGE ANNUAL ETHYLENE DIBROMIDE CONCENTRATIONS FOR CITIES WITH POPULATIONS EXCEEDING 1,000,000

City	SMSA population, 10^3	City population, 10^3	City area, $10^9 m^2$	Automobile registration	Emission rate 10^{-10} g/s-m²	Wind speed, m/s	EDB[b] concentration Central city 10^{-3} µg/m³	Central city ppt	Suburban 10^{-3} µg/m³	Suburban ppt
Chicago	6,998.8	3,173	0.57	1,324,171	3.71	5	16	2.1	6.6	0.9
Detroit	4,446.3	1,387	0.35	675,065	3.08	6	11	1.4	7.7	1.0
Houston	2,163.4	1,320	1.1	701,766	1.01	6	4	0.5	0.74	0.1
Los Angeles	6,938.3	2,747	1.2	1,490,483	1.98	3	14	1.8	3.0	0.4
New York	9,746.4	7,647	0.77	1,707,891	3.54	7	11	1.4	1.8	0.2
Philadelphia	4,826.3	1,862	0.33	944,660	4.57	6	17	2.2	1.0	0.1

[a] Assumes 80 percent of vehicles use leaded gasoline.
[b] Ethylene dibromide.

Source: SRI International, 1978.

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TABLE E-34. RESULTS OF ETHYLENE DIBROMIDE MONITORING IN THE
VICINITY OF MANUFACTURING FACILITIES

Company	Location	Number of sites[a]	Total sampling time,[b] h	Concentration,[c] ppb	Standard deviation
Dow	Magnolia, Ark.	1	4	13.2	0.9
Ethyl Corp.	Magnolia, Ark.	1	8	3.1	4.3

[a]All sites were within 100 m of the plant.

[b]Samples were discontinuous; two were taken near the Dow facility and five
near the Ethyl Corporation facility.

[c]To convert to $\mu g/m^3$, divide by 0.13.

Source: SRI International, 1978.

TABLE E-35. ESTIMATES OF ETHYLENE DIBROMIDE EXPOSURES FROM
SELF-SERVICE GASOLINE PUMPS

Customer	Nozzle time, min	Gallons pumped	Estimated EDB[a] level	
			$\mu g/m^3$	ppt
1	2.5	14	0.345	45
2	1.1	8	0.972	126
3	1.6	9	5.220	679

Average Nozzle Time = 1.7 min.
Time-weighted average exposure = 260 ppt.

[a]Ethylene dibromide.

Source: SRI International, 1978. The conversion is based on differences in
vapor pressure and concentration between benzene and ethylene
dibromide in gasoline.

Storage and Transportation:
Protection against physical damage is required. Should be stored in cool, dry, well-ventilated location, away from any area where the fire hazard may be acute. Shipped in glass bottles, metal drums, and tank cars.

Disposition:
Ethylene dibromide may be disposed of by controlled incineration with adequate scrubbing and ash disposal facilities.

Sampling and Analytical Methods

1. NIOSH Method 1008
   a. Solid Sorbent Tube (coconut shell charcoal, 100 mg/50 mg).
   b. Gas chromatography, electron capture detector.

   Detection limit:
   0.04 mg/m³ per 25-liter sample

   Possible interferences:
   None idnetified.

2. NIOSH Method S104
   a. Adsorption with charcoal.
   b. Desorption with carbon disulfide.
   c. Gas chromatography.

   Detection limit:
   22 to 660 mg/m³ per 1-liter sample

   Possible interferences:
   Any compound that has the same retention time may inter-fere. High humidity.

Permissible Exposure Limits

	OSHA	ACGIH	NIOSH
TWA	20 ppm		
Ceiling	30 ppm	none	1 mg/m³ (15 min)
Peak	50 ppm (5 min)		

The ACGIH lists ethylene dibromide as an industrial substance suspected of carcinogenic potential for man (skin).

Human Toxicity

Acute Toxicity:
Severe skin irritant. Serious toxic interaction between inhaled ethylene dibromide and ingested disulfiram. One case of fatal poisoning reported after ingestion of 4.5 ml.

Patient vomited recurrently, had watery diarrahea, became
anuric, and died 2 days later. Massive damage of the kidneys
noted at autopsy.

Chronic Toxicity:
Both the National Cancer Institute and the National Toxicology
Program have found ethylene dibromide to be carcinogenic in
both mice and rats; therefore, it can be considered a
suspected human carcinogen.

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Chemical Name

Ethylene oxide

CAS Number

65-21-8

Chemical Classification

Epoxide

Synonyms

Aethylenoxid; anprolene; benvicide; carboxide; cry-oxide; di-hydroxirene; dimethylene oxide; E.O.; 1,2-epoxyacthan; epoxyethane; 1,2-epoxyethane; ethyleen oxide; ethylene oxide (DOT); ethylene (oxide'd); etilene (ossido di); ETO; eto; etylenutlener; NCI-C50088; oxacyclopropane; oxane; oxidoethane; alpha-beta-oxidoethane; oxiraan; oxiran; oxirane; oxirene, dihydro-; oxyfume 12; oxyfume sterilant 20; pennoxide, steroxide 12; steroxide 20; t-gas;

Physical/Chemical Properties

Description:
Colorless gas at room temperature. Ether-like odor over 700 ppm.

Boiling Point:
10.73°C

Melting Point:
-111.3°C

Molecular Weight:
44.1

Chemical Formula:
CH_2CH_2O

Vapor Pressure:
1095 mm at 20°C

Vapor Density:
1.52 (air = 1)

Refractive Index:
$N_D^7 = 1.3597$

Solubility:
Soluble in organic solvents; miscible with water in all pro-portions.

Log Partition Coefficient (octanol/water):
   -0.3

Photochemical Reactivity:
   Reactivity toward OH· is the same as butane. No reaction
   toward photolysis.

Chemical Reactivity:
   Reacts readily with proton donors such as alcohols, amines and
   thiols. Decomposes violently at temperatures above 800°C.
   Ethylene oxide will polymerize violently if contaminated with
   aqueous alkalies, amines, mineral acids, metal chlorides, or
   metal oxides. Incompatible with alkalines and acids. Reacts
   with active hydrogen compounds (e.g., alcohols, amines, and
   sulphydryl compounds) and with inorganic chloride in food to
   form ethylene chlorohydrin. Also reacts with 4-4'-nitrobenzyl
   pyridine.

Environmental Fate

In connection with the treatment of foods with ethylene oxide, the
compound reacts with inorganic chloride to form ethylene
chlorohydrin.

Source of Emissions

Production:
   From oxidation of ethylene in air or oxygen with silver cata-
   lyst.
   From the reaction of ethylene with hypochlorous acid followed
   by dehydrochlorination of the resulting chlorohydrin with lime
   (chlorohydrin process).

Uses:
   Manufacture of ethylene glycol and higher glycols
   Surfactants
   Acrylonitrile
   Ethanolamines
   Petroleum demulsifier
   Fumigant
   Rocket propellant
   Industrial sterilant, e.g., medical plastic tubing
   Fungicide

   Tables E-36 through E-41 and Figure E-2 present data on ethyl-
   ene oxide production, consumption, and emissions.

Storage:
   Should be protected against physical damage. Should be kept
   cool, below 86°F. Should be stored outside, away from build-
   ings and other materials, in insulated tanks or containers,
   shielded from sun and heat or provided with cooling facilities
   and protected by a properly designed water-spray system.

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TABLE E-36. ETHYLENE OXIDE PRODUCERS

Source	Location	Type of process[a]	1978 estimated production,[b] 10^6 lb/yr	1978 estimated capacity, 10^6 lb/yr	Geographic coordinates
BASF Wayandotte	Geismar, LA	B	222	310	30 11 34/91 00 42
Celanese	Clear Lake, TX	B	340	475	29 37 17/95 03 51
Dow	Freeport, TX	A	322	450	28 59 15/95 24 45
	Plaquemine, LA	A	351	490	30 19 00/91 15 32
Jefferson Chemical	Port Neches, TX	A	340	475	29 57 45/93 56 00
Northern Petrochemical	East Morris, IL	B	165	230	41 24 08/88 17 18
Olin	Brandenburg, KY	B	75	105	38 00 27/86 06 50
PPG	Beaumont, TX	B	107	150	30 03 40/94 02 30
Shell Chemical	Geismar, LA	B	193	270	30 11 00/90 59 00
Sunolin Chemical	Claymont, DE	B	72	100	39 48 20/75 25 40
Texas Eastman	Longview, TX	B	136	190	32 25 55/94 41 06
Union Carbide	Seadrift, TX	A	594	830	28 30 31/96 46 18
	Taft, LA	A	723	1010	29 58 00/97 27 00
Total			3640	5085	

[a]A = air oxidation process.
  B = oxygen oxidation process.

[b]The distribution of production for each producer is determined by the ratio of total U.S. production/
total capacity times individual site capacity.

Source: Systems Applications, Inc. 1980.

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TABLE E-37. ETHYLENE OXIDE PRODUCERS AND USERS

Source	Location	1978 capacity (lb × 10^6)					
		Ethylene oxide	Ethylene glycol	Diethylene glycol	Triethylene glycol	Glycol ethers	Ethanol-amines
BASF Wayandotte	Geismar, LA	310		20		230	
Celanese	Clear Lake, TX	475		50	10		
Dow	Freeport, TX / Plaquemine, LA	450 / 490	330 / 550	25 / 50	50		40 / 100
Jefferson	Port Neches, TX	475	360	35	20	40	80
Northern Petrochemical	East Morris, IL	230	350	35			
Olin	Brandenburg, KY	105	50	5	2	70	25
PPG	Beaumont, TX	150	200	20		20	
Shell Chemical	Geismar, LA	270	200	20	5	50	
Sunolin Chemical	Claymont, DE	100					
Texas Eastman	Longview, TX	190	180	20		25	
Union Carbide	Seadrift, TX / Taft, LA	830 / 1010	870 / 1200	80 / 100	75[a]	490[a]	230
ICI Americas	Hopewell, VA		33				

[a]Includes a plant in Penuelas, Puerto Rico.

Source: Systems Applications, Inc. 1982.

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TABLE E-38. END-USE DISTRIBUTION OF ETHYLENE OXIDE IN 1978

	Usage	
	10^6 lb/yr	%
Ethylene glycol polyester	910	25
Ethylene glycol antifreeze	837	23
Ethylene glycol (other uses)	364	10
Surface active agents	546	15
Ethanolamines	255	7
Glycol ethers	255	7
Other	473	13
Total	3640	100

Source: Systems Applications, Inc., 1980.

TABLE E-39. ESTIMATED 1978 NATIONWIDE EMISSIONS OF ETHYLENE OXIDE

Source	Production/ usage 10⁶ lb/yr	Usage %	Total emissions	
			lb/yr	g/s
Producers[a]				
Air oxidation	2330		1,277,000	18.4
Oxygen oxidation	1310		410,900	5.9
Users				
EG[b] polyester	910	25		
EG antifreeze	837	23		
EG (other uses)	364	10		
Surface active agents	546	15		
Ethanolamines	255	7		
Glycol ethers	255	7		
Other	473	13		
Total			1,687,900	24.3

[a]Total emissions from producers also include total emissions from users since ethylene oxide is produced and used at the same site.

[b]EG = ethylene glycol.

Source: Systems Applications, Inc., 1982.

TABLE E-40. ETHYLENE OXIDE EMISSIONS FROM PRODUCERS
(Air Oxidation Process)

Company	Location	Process emissions, lb	Storage emissions, lb	Fugitive emissions, lb	Total emissions	
					lb	g/s
Dow	Freeport, TX Plaquemine, LA	169,000 184,000	6,880 7,500	529 577	176,000 192,000	2.5 2.8
Jefferson	Port Neches, TX	179,000	7,270	559	187,000	2.7
Union Carbide	Seadrift, TX Taft, LA	312,000 380,000	12,700 15,500	977 1,190	326,000 397,000	4.7 5.7
Total		1,224,000	49,850	3,832	1,278,000	18.4

Source: Systems Applications, Inc. 1982.

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TABLE E-41. ETHYLENE OXIDE EMISSIONS FROM PRODUCERS
(Oxygen Oxidation Process)

Company	Location	Process emissions, lb	Storage emissions, lb	Fugitive emissions, lb	Total emissions	
					lb	g/s
BASF	Geismar, LA	1,032	156	12	1,200	.02
Celanese	Clear Lake, TX	135	12	1,853	2,000	.03
Northern Petrochemical	Port Neches, TX	77,340	11,690	899	89,930	1.3
Olin	Brandenburg, KY	35,150	5,314	409	40,880	0.6
PPG	Beaumont, TX	50,150	7,581	583	58,320	0.8
Shell Chemical	Geismar, LA	90,460	13,670	1,052	105,200	1.5
Sunolin Chemical	Claymont, DE	33,750	5,101	392	39,240	0.6
Texas Eastman	Longview, TX	63,740	9,636	741	74,120	1.1
Total		351,667	53,158	5,942	410,900	5.9

Source: Systems Applications, Inc. 1982.
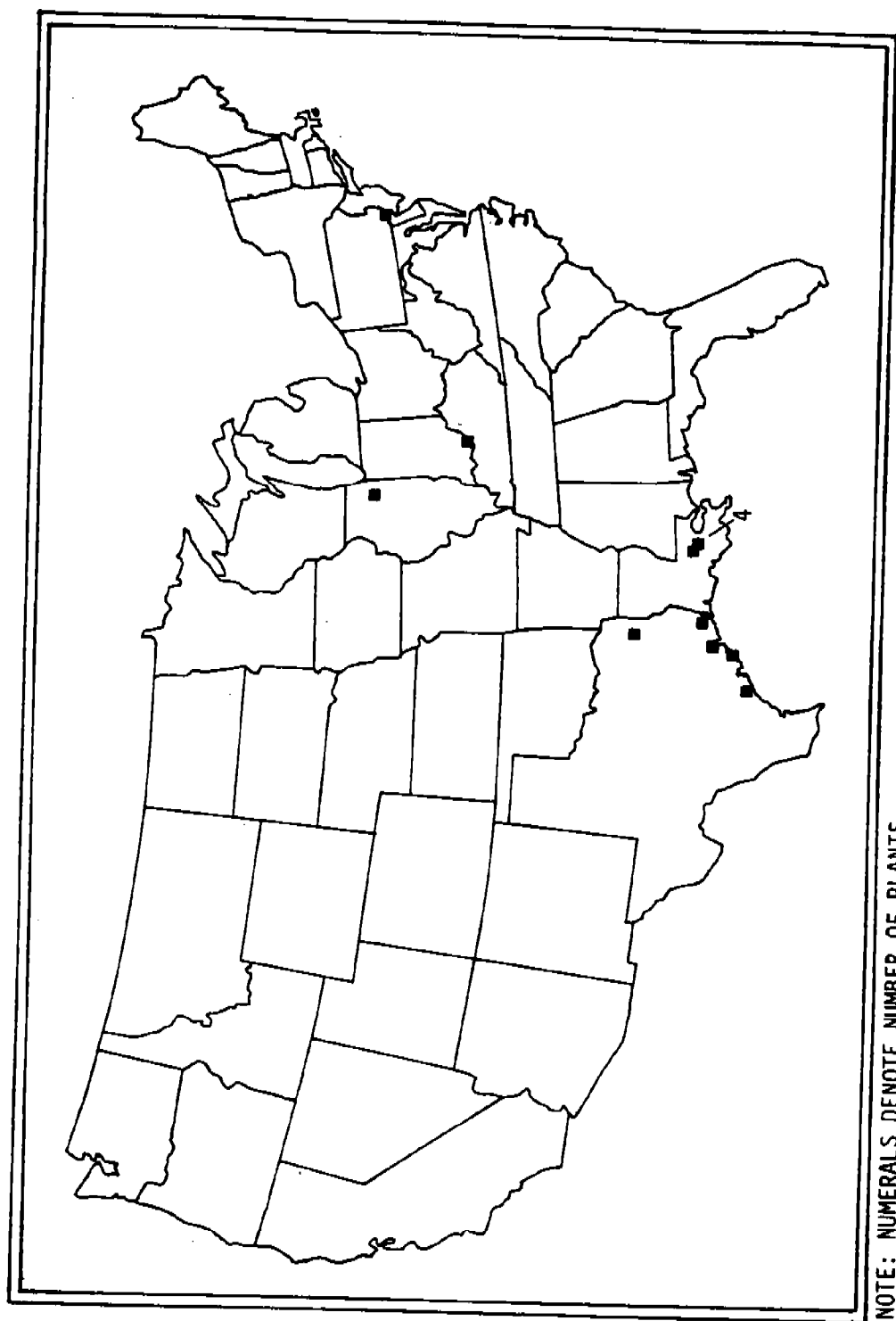
Figure E-2. Specific point sources of ethylene oxide emissions

Source: Systems Applications, Inc. 1980.

NOTE: NUMERALS DENOTE NUMBER OF PLANTS.

Adequate diking and drainage should be provided in tank area
to confine and dispose of liquid in case of a tank rupture.
Pits and depressions should be avoided. Inside storage should
be held at a minimum and confined to a standard fire-resistant
flammable liquids storage room, provided with continuous
ventilation and free of sources of ignition.

Transportation:
Shipped in steel cylinders, drums, insulated tank cars, and
tank barges. The U.S. Bureau of Explosives requires a red
label on all shipments. Not acceptable on passenger planes.

Disposition:
Ethylene oxide may be disposed of as a concentrated waste
containing no peroxide by discharging liquid at a controlled
rate near a pilot flame or as a concentrated waste containing
peroxides by perforation of a container of the waste from a
safe distance followed by open burning. Ethylene oxide is a
hazardous waste with a hazardous waste number of U 115 as-
signed by EPA.

Sampling and Analytical Methods

1. NIOSH Method S286
    a. Adsorption on charcoal.
    b. Desorption with carbon disulfide.
    c. Gas chromatography.

    Detection limit:
        20 to 270 mg/m³ for a 5-liter sample.

    Possible interferences:
        High humidity. Any compound with the same retention time
        may cause an interference.

2. Method A (Appendix A)
    a. Direct gas injection into gas chromatograph/flame.
    b. Ionization detector.

    Detection limit:
        0.01 ppm

    Possible interferences:
        Losses from surface adsorption may occur in some cases.

3. Method B (Appendix A) C_2-C_{18} hydrocarbons and other nonpolar
    organics with a boiling point of 100° to 175°C
    a. Whole air collection in canister.
    b. Cryogenic concentration.
    c. Gas chromatography/flame ionization detection.

    Detection limit:
        0.1 ppb per 100-ml sample

Possible interferences:
Water soluble compounds are not readily analyzed. Storage times greater than a week are not recommended.

4. Method E (Appendix A)
   a. Adsorption on charcoal.
   b. Desorption with CS_2.
   c. Analysis by gas chromatography/flame ionization detection.

Detection limit:
0.1 to 1 ppm per 10-liter sample

Possible interferences:
Sensitivity much poorer than for thermal desorption.

Permissible Exposure Limits

	OSHA	ACGIH
TWA	1 ppm	1 ppm (2 mg/m^3)

The ACGIH lists ethylene oxide as an industrial substance suspected of carcinogenic potential for man.

Human Toxicity

Acute Toxicity:
Powerful irritant (systemic). High toxicity effect through oral, inhalation, intraperitoneal, and intravenous means. An irritant to skin, eyes, and mucous membranes of respiratory tract. High concentrations can cause pulmonary edema.

Chronic Toxicity:
Tests on rats found ethylene oxide to be an equivocal tumorigenic agent. Currently tested by the National Toxicology Program for carcinogenesis bioassay.

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Chemical Name

Formaldehyde

CAS Number

50-00-0

Chemical Classification

Aldehyde

Synonyms

Aldehyde formique; aldehyde formica; BFV; FA; fannoform; formaldehyd; formaldehyde, as formalin solution (DOT); formalin-loesungen; formalith; formicaldehyde; formel; FYDE; hoch; ivalon; karsan; cysoform; methanal; methylaldehyde; methylene glycol; methylene oxide; morbicide; NCI-C02799; opplossingen; oxomethane; oxymethylene; paraform; polyoxymethylene glycols; superlysoform; tetraoxynethylene; trioxane

Physical/Chemical Properties

Description:
Gas; strong pungent odor.

Boiling Point:
-19°C

Melting Point:
-118°C

Molecular Weight:
30.0

Chemical Formula:
HCHO

Vapor Pressure:
760 mm at -19.5°C

Vapor Density:
1.067 (air = 1)

Refractive Index:
Not available

Solubility:
Soluble in water and alcohol.

Log Partition Coefficient (octanol/water):
    -0.96

Photochemical Reactivity:
    Reactivity toward OH· is 2 to 4 times butane. Photolysis is 9 percent per hour at full sunlight. Major atmospheric precursors are hydrocarbons (photooxidation). Formed by incomplete combustion of many organic substances. Equilibrium is approximately 5 percent for methane hydrocarbons.

Chemical Reactivity:
    Reacts with NO_x at about 180°F, when the reaction becomes explosive. Also reacts violently with HlO_4-aniline and performic acid, nitromethane, magnesium carbonate, and hydrogen peroxide. Can react with hydrogen chloride and inorganic chlorides to yield bis-chloromethyl ether (BCME) which is a potent carcinogen. This reaction occurs only at high (500 to 3,000 ppm) concentrations.

Environmental Fate
        Bioaccumulation of formaldehyde is unlikely due to its high chemical reactivity. Degradation in the atmosphere is by photochemical process, and it biodegrades to formic acid, methyl alcohol, carbon dioxide, and water.

Source of Emissions

    Production:
        Oxidation of synthetic methanol or low boiling petroleum gases such as propane and butane. The most common catalysts are silver, copper, or iron-molybdenum.

    Uses:
        Urea and melamine resins
        Polyacetal resins
        Phenolic resins
        Ethylene glycol
        Pentaerythritol
        Hexamethylenetetramine
        Fertilizer
        Dyes, medicine (disinfectant, germicide)
        Embalming fluids
        Preservative
        Hardening agent
        Reducing agent, as in recovery of gold and silver
        Corrosion inhibitor in oil wells
        Durable-press treatment of textile
        Industrial sterilant
        Treatment grain

        Tables E-42 through 4-46 and Figure E-3 present formaldehyde production, consumption and emission data.

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TABLE E-42. PRODUCTION OF FORMALDEHYDE

Source	Location	1978 Estimated production,[a] 10^6 lb/yr	1978 Estimated capacity, 10^6 lb/yr	Geographic coordinates, Latitude/longitude
Allied Chemical	South Point, OH	222	310	38 25 43/82 36 00
Borden, Inc.	Demopolis, AL	72	100	32 30 48/27 50 06
	Diboll, TX	57	80	31 11 52/94 46 50
	Fayetteville, NC	168	235	35 01 43/78 51 41
	Geismar, LA	179	250	30 13 00/91 01 00
	Louisville, KY	57	80	38 12 09/85 51 49
	Sheboygan, WI	93	130	43 45 26/87 46 17
	Fremont, CA	161	225	37 32 06/121 57 24
	Kent, WA	57	80	47 23 12/122 13 15
	LaGrande, OK	46	65	45 20 31/100 02 02
	Missoula, MT	64	90	46 54 10/114 40 00
	Springfield, OR	172	240	44 02 60/122 59 06
Celanese Chemical	Bishop, TX	1075	1500	27 34 06/97 49 27
	Newark, NJ	84	117	40 43 30/74 07 25
	Rock Hill, SC	84	117	34 57 25/80 57 32
Chembond Corp.	Springfield, OR	107	150	44 02 60/122 59 06
	Winnifield, LA	50	70	31 54 49/92 40 35
Du Pont	Belle, WV	358	500	38 12 13/81 28 34
	LaPorte, TX	229	320	29 42 04/95 02 05
	Healing Springs, NC	158	220	35 01 56/80 10 30
	Linden, NJ	115	160	40 36 02/74 12 08
	Toledo, OH	193	270	41 39 22/83 33 20
GAF Corp.	Calvert City, KY	72	100	37 02 50/88 21 12

(continued)

TABLE E-42 (continued)

Source	Location	1978 Estimated production, 10^6 lb/yr[a]	1978 Estimated capacity, 10^6 lb/yr	Geographic coordinates, Latitude/longitude
Georgia-Pacific Corp.	Albany, OR	86	120	44 37 07/123 05 13
	Columbus, OH	72	100	39 53 07/82 56 45
	Coosbay, OR	65	90	42 27 26/124 10 47
	Crossett, AR	115	160	33 08 36/93 02 11
	Russelville, SC	143	200	33 20 52/79 58 00
	Taylorsville, MS	86	120	39 51 00/89 25 00
	Vienna, GA	72	100	37 07 30/83 49 00
	Lufkin, TX	72	100	31 21 00/94 47 00
Gulf Oil Corp.	Vicksburg, MS	43	60	32 17 00/90 54 00
Hercules Inc.	Louisiana, MO	122	170	39 26 24/91 03 37
	Wilmington, NC	72	100	34 19 09/77 59 23
Hooker Chemicals & Plastics	Tonawanda, NY	97	135	43 02 47/78 51 44
IMC Chemical Group	Seiple, PA	47	65	40 38 12/75 31 58
	Sterlington, LA	22	30	32 43 25/92 08 56
Monsanto Corp.	Addyston, OH	72	100	39 07 30/84 42 58
	Chocolate Bayou, TX	140	195	29 14 55/95 12 45
	Eugene, OR	72	100	44 02 59/123 08 19
	Springfield, MA	211	295	42 09 33/72 29 09
Pacific Resins and Chemicals	Eugene, OR	68	95	44 01 00/123 05 05

(continued)

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TABLE E-42 (continued)

Source	Location	1978 Estimated production, 10^6 lb/yr[a]	1978 Estimated capacity, 10^6 lb/yr	Geographic coordinates, Latitude/longitude
Reichhold Chemicals, Inc.	Hampton, SC	36	50	32 53 33/81 06 10
	Houston, TX	86	120	29 44 50/95 10 00
	Kansas City, KA	36	50	39 09 28/94 37 41
	Malvern, AR	79	110	34 24 09/92 48 45
	Moncure, NC	86	120	35 31 18/79 04 52
	Tacoma, WA	36	50	47 16 11/122 22 57
	Tuscaloosa, AL	50	70	33 12 03/87 34 00
	White City, OR	179	250	42 26 18/122 07 07
Tenneco, Inc	Fords, NJ	133	185	40 30 50/74 19 17
	Garfield, NJ	72	100	40 52 28/74 06 49
Wright Chemical Corp.	Riegelwood, NC	57	80	34 19 22/78 12 09
		6,400	8,929	

[a]The distribution of production for each producer is determined by the ratio of total U.S. production to total U.S. capacity as compared to individual plant opacity.

Source: System Applications, Inc. 1982.

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TABLE E-43. FORMALDEHYDE CONSUMPTION BY END USE

End-Use	Percent of total consumption	End-use consumption 10^6 lb/yr
Urea resins	25.4	1630
Phenolic resins	24.3	1560
Butanediol	7.7	490
Acetal resins	7.0	450
Pentaerythritol	6.0	380
Hexamethylenetetramine	4.5	290
Melamine resins	4.2	270
Urea formaldehyde concentrates	3.6	230
Chelating agents	3.6	230
Trimethylolpropane	1.3	80
Other Chemical intermediate uses	11.9	760
Export	0.5	30
Total	100.0	6400

TABLE E-44. FORMALDEHYDE CHEMICAL INTERMEDIATE USERS

Source	Location	1978 Estimated formaldehyde consumption, 10^6 lb	Geographic coordinates, Latitude/longitude
Butanediol Production			
Du Pont Company	Houston, TX	240	29 42 04/95 02 05
GAF Corporation	Calvert City, KY	80	37 02 50/88 21 12
	Texas City, TX	80	29 25 29/94 58 07
Total		400	
Acetal Resins Production			
Celanese Corporation	Bishop, TX	310	27 34 06/97 49 27
Du Pont Company	Parkersburg, WV	140	39 15 27/81 32 52
Total		450	
Pentacrythritol Production			
Celanese Corporation	Bishop, TX	160	27 34 06/97 49 27
Hercules, Inc.	Louisiana, MO	100	39 26 24/91 03 37
IMC (CSC)	Seiple, PA	50	40 38 12/75 31 58
Perstop AB	Toledo, OH	70	41 42 33/83 30 00
Total		380	
Hexamethylenetetramine Production			
Borden, Inc.	Fayetteville, NC	60	35 01 43/78 51 41
W. R. Grace & Company	Nashua, NH	60	42 46 00/71 27 52
Occidental Petroleum Co.	North Tonawanda, NY	50	43 02 47/78 51 44
Plastics Engineering Co.	Sheboygan, WI	20	43 45 00/87 47 00
Tenneco, Inc.	Fords, NJ	40	40 30 50/74 19 17
Wright Chemical Corp.	Acme, NC	60	34 19 22/78 12 09
Total		290	
Trimethylolpropane Production			
Celanese Corp.	Bishop, TX	80	27 34 06/97 49 27

Source: System Applications, Inc. 1982.

TABLE E-45.   1978 FORMALDEHYDE PRODUCTION EMISSIONS

Company	Location	1978 production, 10^6 lb	Type of process	Process emissions, 10^4 lb	Storage emissions, 10^4 lb	Fugitive emissions, 10^4 lb	Total emissions 10^4 lb	Total emissions g/s
Allied Chemical	South Point, OH	222	A	5.81	0.46	0.91	7.19	1.04
Borden, Inc.	Demopolis, AL	72	A	1.89	0.15	0.30	2.33	0.34
	Diboll, TX	57	A	1.49	0.12	0.23	1.85	0.27
	Fayetteville, NC	168	A	4.40	0.35	0.69	5.44	0.78
	Geismar, LA	179	A	4.69	0.37	0.74	5.79	0.83
	Louisville, KY	57	A	1.49	0.12	0.23	1.85	0.27
	Sheboygan, WI	93	A	2.44	0.19	0.38	3.01	0.43
	Fremont, CA	161	A	4.22	0.33	0.66	5.21	0.75
	Kent, WA	57	A	1.49	0.12	0.23	1.85	0.27
	LeGrande, OR	46	A	1.21	0.09	0.19	1.49	0.21
	Missoula, MT	64	A	1.68	0.13	0.26	2.07	0.30
	Springfield, OR	172	A	4.51	0.35	0.71	5.57	0.80
Celanese Chemical	Bishop, TX	1075	A	8.84	0.70	1.36	10.98	1.58
	Newark, NJ	84	B	3.30	0.43	0.68	4.41	0.63
	Rock Hill, SC	84	B	3.30	0.43	0.68	4.41	0.63
Chembond Corp.	Springfield, OR	107	B	4.20	0.55	0.86	5.62	0.81
	Winnfield, LA	50	B	1.96	0.26	0.40	2.62	0.38
Du Pont	Belle, WV	358	A	9.38	0.74	1.47	11.59	1.67
	LaPorte, TX	229	A	6.00	0.47	0.94	7.41	1.07
	Healing Springs, NC	158	A	4.14	0.33	0.65	5.11	0.74
	Linden, NJ	115	A	3.01	0.24	0.47	3.72	0.54
	Toledo, OH	193	A	5.06	0.40	0.79	6.25	0.90
GAF Corp.	Calvert City, KY	72	B	2.83	0.37	0.58	3.78	0.54
Georgia-Pacific Corp.	Albany, OR	86	B	3.38	0.44	0.69	4.51	0.65
	Columbus, OH	72	B	2.83	0.37	0.58	3.78	0.54
	Coos Bay, OR	65	B	2.55	0.34	0.52	3.41	0.06
	Crossett, AR	72	A	0.00	0.15	0.30	0.45	0.08
		43	B	0.00	0.22	0.35	0.57	0.33
	Russelville, SC	143	B	5.61	0.74	1.15	7.51	1.08
	Taylorsville, MS	86	B	3.38	0.44	0.69	4.51	0.65
	Vienna, GA	72	A	0.00	0.15	0.30	0.45	0.06
	Lufkin, TX	72	B	0.00	0.37	0.58	0.95	0.14
Gulf Oil Corp.	Vicksburg, MS	43	B	1.69	0.22	0.35	2.26	0.33
Hercules Inc.	Louisiana, MO	122	A	3.20	0.25	0.50	3.95	0.57
	Wilmington, NC	72	A	1.89	0.15	0.30	2.33	0.34
Hooker Chemicals & Plastics	Tonawanda, NY	97	A	2.54	0.20	0.40	3.14	0.45
IMC Chemical Group	Seiple, PA	47	A	1.23	0.10	0.19	1.52	0.22
	Sterlington, LA	22	A	0.58	0.05	0.09	0.71	0.10

(continued)

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TABLE E-45 (continued)

Company	Location	1978 production, 10^6 lb	Type of process	Process emissions, 10^4 lb	Storage emissions, 10^4 lb	Fugitive emissions, 10^4 lb	Total emissions 10^4 lb	Total emissions g/s
Monsanto Corp.	Addyston, OH	72	A	0.34	0.03	0.05	0.42	0.06
	Chocolate Bayou, TX	140	A	0.66	0.05	0.11	0.82	0.12
	Eugene, OR	72	A	0.34	0.03	0.05	0.42	0.06
	Springfield, MA	211	A	1.00	0.08	0.16	1.23	0.18
Pacific Resins and Chemicals	Eugene, OR	68	A	1.78	0.14	0.28	2.20	0.32
Reichhold Chemicals, Inc.	Hampton, SC	36	A	0.94	0.07	0.15	1.17	0.17
	Houston, TX	86	B	3.38	0.44	0.69	4.51	0.65
	Kansas City, KA	36	A	0.94	0.07	0.15	1.17	0.17
	Malvern, AR	79	B	3.10	0.41	0.64	4.15	0.60
	Moncure, NC	86	B	3.38	0.44	0.69	4.51	0.65
	Tacoma, WA	36	B	1.41	0.19	0.29	1.89	0.27
	Tuscaloose, AL	50	A	1.31	0.10	0.21	1.62	0.23
	White City, OR	179	B	7.03	0.93	1.44	9.40	1.35
Tenneco, Inc	Fords, NJ	71	A	1.86	0.15	0.29	2.30	0.33
	Garfield, NJ	62	B	2.43	0.32	0.50	3.25	0.45
		72	A	1.89	0.15	0.30	2.33	0.34
Wright Chemical Corp.	Riegelwood, NC	57	B	2.24	0.29	0.46	2.99	0.43
Total		6400		150.24	15.76	30.86	193.97	27.92

Source: Systems Applications, Inc., 1982.

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TABLE E-46. FORMALDEHYDE EMISSIONS FROM CHEMICAL INTERMEDIATE USERS

Source	Location	Process emissions, lb/yr	Storage emissions, lb/yr	Fugitive emissions, lb/yr	Total emissions lb/yr	Total emissions g/s
Butanediol Producers						
Du Pont Company	Houston, TX	480,000	120,000	120,000	720,000	10.37
GAF Corporation	Calvert City, KY	160,000	40,000	40,000	240,000	3.46
	Texas City, TX	160,000	40,000	40,000	240,000	3.46
Total		800,000	200,000	200,000	1,200,000	
Acetal Resins Producers						
Celanese Corporation	Bishop, TX	391,409	48,927	48,927	489,263	7.04
Du Pont Company	Parkersburg, WV	560,000	70,000	70,000	700,000	10.08
Total		951,409	118,927	118,927	1,189,263	
Pentacrythritol Producers						
Celanese Corporation	Bishop, TX	369,208	44,445	20,708	434,361	6.25
Hercules, Incorporated	Louisiana, MO	731,000	88,000	41,000	860,000	12.38
IMC (CSC)	Seiple, PA	365,500	44,000	20,500	430,000	6.19
Perstorp AB	Toledo, OH	511,700	61,600	28,700	602,000	8.67
Total		1,977,408	238,045	110,908	2,326,361	
Hexamethylenetetramine Producers						
Borden, Inc.	Fayetteville, NC	63,000	9,000	18,000	90,000	1.30
W. R. Grace & Company	Nashua, NH	63,000	9,000	18,000	90,000	1.30
Occidental Petroleum Company	North Tonawanda, NY	52,500	7,500	15,000	75,000	1.08
Plastics Engineering Company	Sheboygan, WI	21,000	3,000	6,000	30,000	0.43
Tenneco, Inc.	Fords, NJ	42,000	6,000	12,000	60,000	0.86
Wright Chemical Corporation	Acme, NC	63,000	9,000	18,000	90,000	1.30
Total		304,500	43,500	87,000	435,000	
Trimethylolpropane Producers						
Celanese Corporation	Bishop, TX	5,050	757	757	6,565	0.09

Source: Systems Applications, Inc. 1982.

Figure E-3. Specific point sources of formaldehyde emissions.

Source: Systems Applications, Inc., 1980.

NOTE: NUMERALS DENOTE NUMBER OF PLANTS.

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Storage and Transportation:
Pure formaldehyde is not available commercially because of its tendency to polymerize. It is sold as aqueous solutions containing from 37 to 50 percent formaldehyde by weight and varying amounts of methanol.

Should be protected against physical damage. Keep separate from oxidizing and alkaline materials. Indoor storage should be in storage areas having floors pitched toward a trapped drain or in curbed retention areas. Minimum storage temperatures to prevent polymerization range from 83°F for 37 percent formaldehyde containing 0.05 methyalcohol to 29°F for formaldehyde containing 15 percent methylalcohol. Shipped in insulated tank cars and tank trucks; 5- to 55-gallon metal drums, carboys, bottles, and tank barges.

Disposition:
Formaldehyde may be disposed of by incineration. Also, formaldehyde may be recovered from waste waters.

Sampling and Analytical Methods

1. NIOSH Method 3501
   a. Liquid in bubbler (midget bubbler, 15-ml Girard T reagent).
   b. Polarography.

   Detection limit:
   4.6 to 19.8 ppm for 18-liter samples.

   Possible interferences:
   Other volatile aldehydes such as acrylein, crotonaldehyde, benzaldehyde, and products diffusing out of polyvinyl chloride tubing may cause significant interference.

2. NIOSH Method 2502
   a. Solid Sorbent Tube [2-(benzylamino) ethanol or Chromasorb 102 or XAD-2 120 mg/60 mg].
   b. Gas chromatography.
   c. Flame ionization detectors.

   Detection limit:
   0.25 to 4 ppm with 12-liter sample.

   Possible interferences:
   Phenol has almost the same retention time. Acid mists may inactivate the sorbent, leading to inefficient collection of formaldehyde.

3. NIOSH Method 3500
   a. Filter and impingers, 1μm PTFE membrane and two impingers, each with 20 ml 1 percent sodium bisulfite solution.
   b. Visible absorption spectrophotometry.

Detection limit:
   0.02 to 0.4 ppm for 80-liter sample

Possible interferences:
   Phenols in 8:1 excess produce 10 to 20 percent bias.
   Ethanol and higher M.W. alcohols, olefins, aromatic
   hydrocarbons, and cyclohexanone produce small negative
   interferences. Little interference is seen from other
   aldehydes.

4.   NIOSH Method 235
   a.   Alumina collection.
   b.   Methanol-water elution.
   c.   Spectrophotometric measurement.

Detection limit:
   0.3 to 0.7 ppm in 6-liter sample

Possible interferences:
   Saturated aldehydes give less than 0.01 percent positive
   interference. Phenols cause 10 to 20 percent negative
   interference when present in an 8:1 ratio over formalde-
   hyde ethylene and propylene present in a 10:1 excess over
   formaldehyde give 5 to 10 percent negative interference,
   while 2-methyl-1,3-butadiene in a 15:1 excess over formal-
   dehyde causes a 15 percent negative interference. Cyclo-
   hexanone causes a bleaching of the final color.

5.   Method J (Appendix A)
   a.   Collection in dinitrophenyl hydrazine (DNPH).
   b.   Solvent extraction of DNPH derivitives.
   c.   Reversed phase high pressure liquid chromatography

6.   Method K (Appendix A)
   a.   Collection in 1 percent sodium bisulfate impinger.
   b.   Determination of formaldehyde using chromotropic acid,
        acrolein, and mercuric chloride hexylrecorcinol with gas
        chromatography/flame ionization detection

Detection limit:
   10 to 30 ppb 120-liter sample

Possible interferences:
   High levels of phenols, ethylene, and propylene cause
   negative interferences with formaldehyde.

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Permissible Exposure Limits

	OSHA	ACGIH	NIOSH
TWA	3 ppm		
Ceiling	5 ppm	2 ppm(3 mg/m^3)	1.2 mg/m^3(30 min)
Peak	10 ppm(30 min.)		
Odor per- ception	1 ppm		

The ACGIH has listed formaldehyde for intended changes to delete
the ceiling, to add 1 ppm (1.5 mg/m^3) for a TWA, to add 2 ppm (3
mg/m^3) as an STEL, and to add a notation that formaldehyde is an
industrial substance suspected of carcinogenic potential for man.

Human Toxicity

Acute Toxicity:
Irritant to skin, eyes, and mucous membrane. If swallowed,
causes violent vomiting and diarrhea, which can lead to
collapse. Frequent or prolonged exposure can cause
hypersensitivity leading to contact dermatitis. Irritant to
eyes at 20 ppm.

Chronic Toxicity:
After reviewing scientific data and public comments relevant
to formaldehyde, EPA has determined there may be a reasonable
basis to conclude that certain exposures to formaldehyde
present or will present a significant risk of widespread harm
to human beings from cancer.

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Chemical Name

Hexachlorocyclopentadiene

CAS Number

77-47-4

Chemical Classification

Chlorinated aromatic

Synonyms

C-56; 1,3-cyclopentadiene, 1,2,3,4,5,5 hexachloro-HCCPD; hexachlorcyklopentadien; hexachlorocyclopentadiene; NCI-C55607. perchlorocyclopentadiene.

Physical/Chemical Properties

Description:
     Pale yellow liquid; pungent odor.

Boiling Point:
     239°C

Melting Point:
     -9.6°C

Molecular Weight:
     272.8

Chemical Formula:
     C_5Cl_6

Vapor Pressure:
     0.4 mm Hg at 50°C; 7.5 mm Hg at 100°C

Vapor Density:
     9.42 (air = 1)

Refractive Index:
     N_D^{25} = 1.563

Solubility:
     Not available

Log Partition Coefficient (Octanol/water):
     3.99

Photochemical Reactivity:
     Not available

Chemical Reactivity:
    When heated to decomposition, emits toxic fumes of chloride.
    Incompatible with sodium.

Environmental Fate
    Important processes for the fate of HCCPD are near-surface photoly-
    sis, adsorption onto organic matter, and possible acid-catalyzed
    hydrolysis to tetrachlorocyclopentadiene if HCCPD is adsorbed onto
    a clay surface. HCCPD bioaccumulated in many organisms with weak
    biodegradation to tetrachlorocyclopentadienone hydrate occurring.

Source of Emissions

Production:
    Mixed pentanes are chlorinated to polychlorinated pentanes in
    the liquid phase followed by vapor phase chlorinalysis and
    ring closure over a surface-active catalyst.

Uses:
    Intermediate for resins, dyes, pesticides, fungicides, pharma-
    ceuticals, and flame retardants.

    Tables E-47 through E-51 and Figure E-4 present data on
    hexachlorocyclopantadiene production, consumption, and emis-
    sions.

Storage:
    Sold as a distilled liquid of high purity in 55-gallon lined
    drums and in tank cars. Not corrosive to most materials of
    construction if moisture is rigorously excluded. To avoid
    possibility of iron contamination and corrosion, glass, nickel,
    or baked phenolic coatings are recommended.

Transportation:
    Transported in lined 55-gallon drums or by tank car.

Disposition:
    Hexachlorocyclopentadiene may be disposed of by incineration
    after it is mixed with another combustible fuel. Care must be
    taken to assure complete combustion to prevent the formation
    of phosgene. An acid scrubber is required to remove the
    halo-acids produced.

Sampling and Analytical Methods

1. NIOSH Method 308
    a. Adsorption on Propak T.
    b. Desorption with hexane.
    c. Gas chromatography.
    d. Electron capture detector.

TABLE E-47. PRODUCTION OF HEXACHLOROCYCLOPENTADIENE

Source	Location	1978 Estimated production[a] (10^6 lb/yr)	1978 Estimated capacity (10^6 lb/yr)	Geographic coordinates latitude/longitude
Hooker Chemical & Plastics Corp.	Montague, MI	1.75	NA[b]	43 24 45/86 22 30
	Niagara Falls, NY	3.50	NA	43 04 52/79 00 34
Velsicol Chemical Corporation	Memphis, TN	1.75	NA	35 09 50/90 57 45
Total		7	NA	

[a]Individual site production allocated by the ratio of the total number of employees at each site compared with the total number of employees at all three sites.

[b]Not available.

Source: Systems Applications, Inc. 1980.

TABLE E-48. HEXACHLOROCYCLOPENTADIENE DERIVATIVES

Compound	End-use category	1974 production, 10^6 lb	1978 Status	Known producer	Location
Aldrin	Pesticides	6.5	No longer made		
Chlorodane	Pesticide	21.2	N/A[a]	Velsicol	Marshall, IL
Dieldrin	Pesticide	1.0	No longer made		
Endosulfan	Pesticide	1.5	N/A	FMC & Hooker	New York, NY
Endrin	Pesticide	1.2	No longer made		
Heptachlor	Pesticide	2.0	N/A	Velsicol	Memphis, TN
Pentac[R]	Pesticide	N/A	No longer made		
Het-acid	Flame retardant	N/A	N/A	Hooker	Niagara Falls, NY
Mivex	Pesticide	N/A	No longer made		
Het-anhydride	Flame retardant	7.0	N/A	Hooker	Niagara Falls, NY
Dichlorane plus	Flame retardant	N/A	N/A	Hooker	Niagara Falls, NY
Chlorendic diesters	Resins	N/A	N/A	Velsicol	Memphis, TN

[a]Not available.

Source: Systems Applications Inc. 1980.

TABLE E-49. 1978 HEXACHLOROCYCLOPENTADIENE PRODUCTION EMISSIONS

Company	Location	Process emissions		Storage emissions		Fugitive emissions		Total emissions	
		lb/yr	g/s	lb/yr	g/s	lb/yr	g/s	lb/yr	g/s
Hooker	Montague, MI	9,100	0.131	1,400	0.020	3,500	0.050	14,000	0.202
	Niagara Falls, NY	18,200	0.262	2,800	0.040	7,000	0.101	28,000	0.404
Velsicol	Memphis, TN	9,100	0.131	1,400	0.020	3,500	0.050	14,000	0.202
Total		36,400		5,600		14,000		56,000	

Source: Systems Applications, Inc. 1980.

TABLE E-50. 1978 HEXACHLOROCYCLOPENTADIENE END-USE EMISSIONS

Company	Location	End-use[a]	Geographic coordinates latitude/longitude	Process emissions lb/yr	Storage emissions lb/yr	Fugitive emissions lb/yr	Total emissions lb/yr	Total emissions g/s
Hooker	Montague, MI	A	43 24 45/86 22 30	570	90	215	875	0.013
	Niagara Falls, NY	A, B	43 04 52/79 00 34	810	125	315	1,250	0.018
Velsicol	Memphis, TN	B, C	35 09 50/90 57 45	390	60	150	600	0.009
	Marshall, IL	A	39 23 00/87 42 30	180	25	70	275	0.004
FMC	Middleport, NY	A	43 12 21/78 29 23	325	50	125	500	0.007
Total				2,275	350	875	3,500	

[a]End-use code: A - pesticide, B - flame retardant, C - resin.

Source: Systems Applications, Inc. 1982.

TABLE E-51. EMISSIONS AND METEOROLOGICAL STATIONS OF SPECIFIC POINT SOURCES OF HEXACHLOROPENTADIENE

No.	Company	Site	Latitude/Longitude	Star station	Plant[a] type	Source[b] type	Emissions g/s		
							Process	Storage	Fugitive
1	Hooker	Montague, MI	43 24 45 086 22 30	14840	1	1 2	.131040 .008208	.020160 .001296	.050400 .003096
2	Hooker	Niagara Falls, NY	43 03 02 079 00 27	14747	1	1 2	.262080 .011664	.040320 .001800	.100800 .004536
3	Velsicol	Memphis, TN	35 09 50 089 57 45	13963	1	1 2	.131040 .005616	.020160 .000864	.050400 .002160
4	Velsicol	Marshall, IL	39 23 00 087 42 30	93819	2	2	.002592	.000360	.001008
5	FMC	Middleport, NY	43 12 21 078 29 23	14747	2	2	.004680	.000720	.001800

[a]Plant types. 1: Plant produces and consumes hexachlorocyclopentadiene; 2: Plant consumes hexachlorocyclopentadiene.

[b]Source types: 1: Hexachlorocyclopentadiene production; 2: Hexachlorocyclopentadiene consumption.
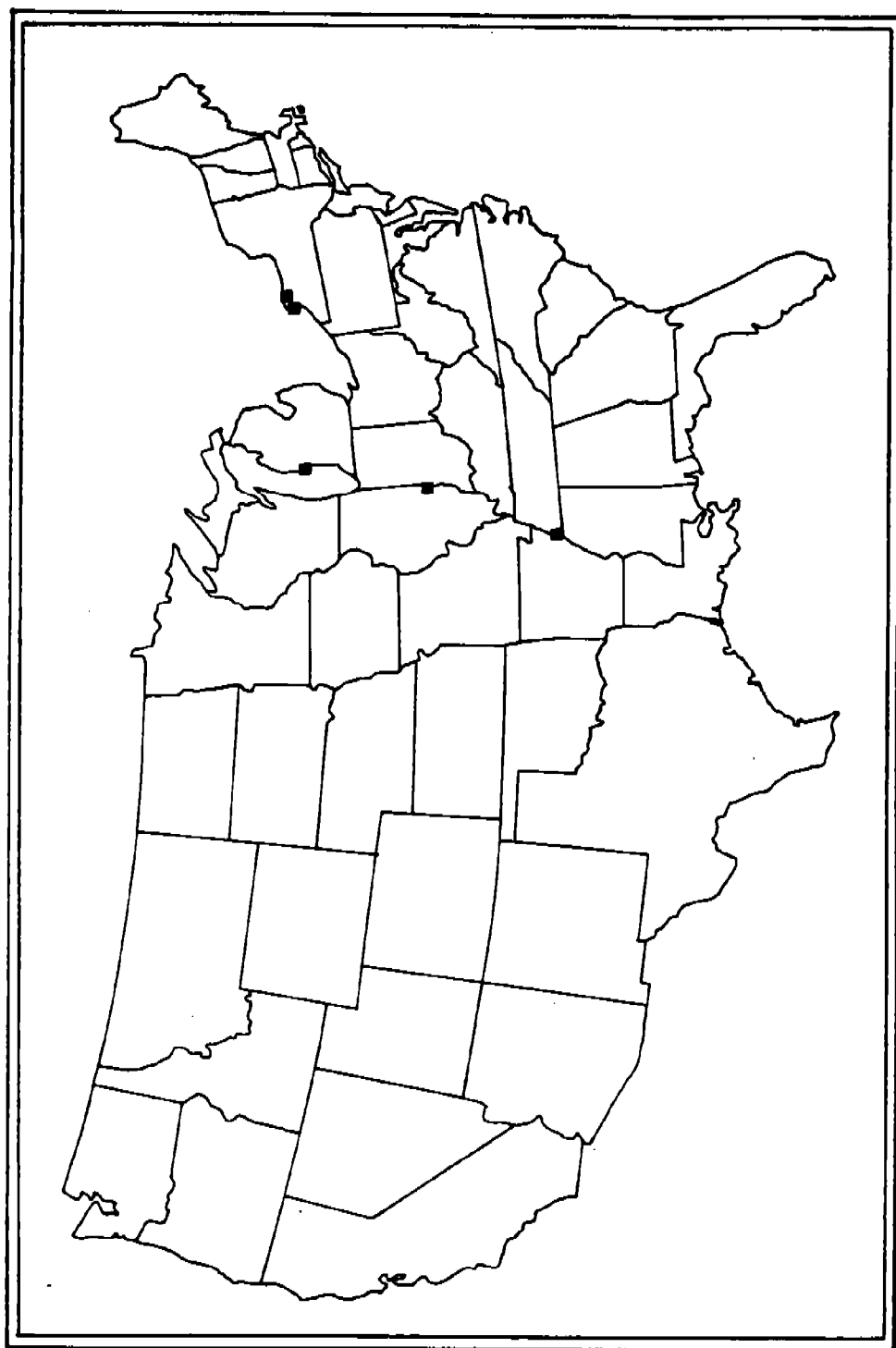
Source: Systems Applications, Inc. 1982.

Figure E-4. Specific point sources of hexachlorocyclopentadiene emissions.

Source: Systems Applications, Inc. 1980.

Detection limit:
      25 ppt

Possible interferences:
      Any compound with the same retention time as
      hexachlorocyclopentadiene at the operating conditions is
      an interferent.

2.   Method C (Appendix A): C_6C_{12} hydrocarbons and other nonpolar
     organics with boiling point between 60° and 200°C.
     a. Adsorption on Tenax.
     b. Thermal desorption.
     c. Gas chromatography/mass spectrometry analysis.

Detection limit:
      1 to 200 ppt for a 20-liter sample

Possible interferences:
      Blank levels usually limit sensitivity artifacts due to
      reactive components (O_3, NO_x). Sample can be analyzed
      only once.

3.   Method D (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar
     organics with boiling point of 60° to 200°C.
     a.   Adsorption on Tenax.
     b.   Thermal desorption into canister.
     c.   Gas chromatography/flame ionization detection, or gas
          chromatography/mass spectrometry analysis.

Detection limit:
      0.01 to 1 ppb for a 20-liter sample

Possible interferences:
      Blanks and artifact problems in Method C, above.

4.   Method H (Appendix A)
     a.   Adsorption on solid adsorbent such as polyurethane foam,
          XAD-2, or Chromasorb 102.
     b.   Solvent desorption.
     c.   Gas chromatography/electron capture detection, gas chro-
          matography/mass spectrometry, or gas chromatography/flame
          ionization detection analysis.

Detection limit:
      3 mg/m³ (1500 m³ sample)

Possible interferences:
      None.

Permissible Exposure Limits

	OSHA	ACGIH
TWA		0.01 ppm (0.1 mg/m^3)
STEL		0.03 ppm (0.3 mg/m^3)

The ACGIH has listed hexachlorocyclopentadiene for intended changes to delete the STEL.

Human Toxicity

Acute Toxicity:
A skin and eye irritant. High oral toxicity. Moderate skin irritant.

Chronic Toxicity:
Selected by the National Toxicology Program for carcinogenesis bioassay as of January 1983.

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Chemical Name

Maleic anhydride

CAS Number

108-31-6

Chemical Classification

Anhydride (unsaturated)

Synonyms

Cis-butenedioic anhydride; 2,5-furandione; maleic acid anhydride; toxilic anhydride

Physical/Chemical Properties

Description:
    Colorless needles

Boiling Point:
    200°C

Melting Point:
    53°C

Molecular Weight:
    98.1

Chemical Formula:
    HC:CH C(O)OC(O)

Vapor Pressure:
    1 mm at 44°C

Vapor Density:
    3.4 (air = 1)

Refractive Index:
    Not available

Solubility:
    Soluble in water, acetone, alcohol, and dioxane; partially
    soluble in chloroform and benzene.

Log Partition Coefficient (octanol/water):
    Not available

Photochemical Reactivity:
    Not available

Chemical Reactivity:
    Dust and vapors are very flammable in air. Reacts violently
    with alkali metals, amines, and other strong oxidizing agents.
    Incompatable with cations or bases. Will react with water or
    steam to produce heat.

Environmental Fate
    Because of its high boiling point and solid state at ambient tem-
    peratures, most maleic anhydride emitted to the air is expected to
    precipitate and be solubilized in water. Conversion to maleic acid
    and subsequent biodegradation is likely to be a major pathway.
    Maleic anhydride in wastewater is easily decomposed by test-acti-
    vated sludge.

Source of Emissions

    Production:
        Vapor phase oxidation of benzene in the presence of vanadium
        oxide catalyst
        Vapor phase oxidation of n-butane in the presence of a
        phosphorous-vanadium catalyst
        Recovery from phthalic anhydride production

    Uses:
        Used exclusively as an intermediate to make:
            Unsaturated polyester resins
            Agricultural chemicals
            Lubricating oil additives
            Copolymers
            Fumaric acid
            Malic acid
            Chlorendic acid and anhydride
            Alkyd resins

        Tables E-52 and E-53 present maleic anhydride production and
        consumption data.

    Storage:
        Should be protected from physical damage and stored in a cool,
        dry, well-ventilated area away from ignition sources; outside
        or detached storage is preferred. Should be protected from
        moisture and stored separately from alkali metals, amines, and
        other strong oxidizing agents. Keep away from flame or spark
        as dust and vapor for molten product are very flammable.

    Transportation:
        Shipped in fiber drums (rod, flake, and lump); iron drums
        (fused); and tank cars (molten).

TABLE E-52. PRODUCTION OF MALEIC ANHYDRIDE

Company	Location	Annual Capacity, 10^6 lb	Raw material and remarks

Ashland Oil, Inc.
  Ashland Chem. Co., Div.
    Petrochems. Div.
  Denka Chem. Corp.
	Neal, W.Va.
	Houston, Tex.
		50
		50
			n-Butane
			n-Butane

Monsanto Co.
  Monsanto Indust.
  Chems. Co.
	Pensacola, Fla.
	St. Louis, Mo.
		130
		110
			n-Butane
			n-Butane (40%); benzene (60%); plant will be converted to 100% butane raw material.

Standard Oil Co. (Indiana) Amoco Chems. Corp., subsid.	Joliet, Ill.	60	n-Butane
United States Steel Corp. USS Chems., div.	Neville Island, Pa.	70	n-Butane (45%); benzene (55%); plant is being converted to 100% butane based feedstock; benzene based capacity is on standby.
	TOTAL	470	

Source: SRI International. 1985.

TABLE E-53. USES OF MALEIC ANHYDRIDE

Use	Millions of pounds (1978)	Percent of total consumption
Unsaturated polyester resins	180	54
Agricultural chemicals	31	9
Lubricating oil additives	30	9
Copolymers	20	6
Fumaric acid	20	6
Malic acid	15	5
Chlorendic acid and anhydride	6	2
Alkyd resins	5	2
All other	24	7
TOTAL	331	100

Source: U.S. EPA 1981 (CHIP)

Disposition:
Maleic anhydride may be disposed of by controlled incinera-
tion. Care must be taken to assure complete oxidation to
non-toxic products.

Sampling and Analytical Methods

1. NIOSH Method 302
    a. Bubbler collection.
    b. High-pressure liquid chromatography.

    Detection limit:
    10 ppb with a 360-liter sample

    Possible interferences:
    Any compound that has the same retention time as maleic
    acid at the process conditions is an interferent. Maleic
    anhydride is immediately hydrolized to maleic acid upon
    -   collection. This method will not differentiate between
    maleic acid and maleic anhydride.

Permissible Exposure Limits

	OSHA	ACGIH
TWA	0.25 ppm (1 mg/m^3)	0.25 ppm (1 mg/m^3)

Human Toxicity

Acute Toxicity:
An eye irritant. Irritation to skin, eyes, and mucous
membranes. Inhalation of vapor can cause pulmonary
edema. Causes burns to skin and eyes.

Chronic Toxicity:
Has been found to be an equivocal tumorigenic agent in
rats. In one study one rat developed two fibrosarcomas
at the site of injection. A mutagenicity test on Chinese
hamster cells was positive for chromosomal aberrations.

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Chemical Name

Manganese

CAS Number

7439-96-5

Chemical Classification

Metallic element

Synonyms

Colloidal manganese; mangan

Physical/Chemical Properties

Description:
Of the four allotropic forms, alpha is the most important.
Brittle reddish-gray, silvery metal.

Boiling Point:
2097°C

Melting Point:
1245°C

Molecular Weight:
54.9

Chemical Formula:
Mn

Vapor Pressure:
1 mm at 1292°C

Density:
7.20

Refractive Index:
Not available

Solubility:
Decomposes in water; readily dissolves in dilute mineral acid.

Log Partition Coefficient (octanol/water):
Not available

Photochemical Reactivity:
No atmospheric transformation (aerosol and particle
deposition). Reacts with all mineral acids with evolution of
hydrogen and formation of divalent manganous salts.

Chemical Reactivity:
>Will react with water or steam to produce hydrogen. Can react with oxidizing materials. Superficially oxidizes on exposure to air. Burns with an intense white light when heated in air.

Environmental Fate

Manganese in the ecosystem has well-established lines of movement from rocks to soils to plants to animals, from soils to water to organisms, and back to water and soils. Marine organisms can concentrate manganese in their bodies, and man retains manganese at a concentration 3 to 4 times that in his food.

Source of Emissions

Production:
>Reduction of the oxide with aluminum or carbon.
>Obtained electrolytically from sulfate or chloride solution.

Uses:
>Ferroalloys (steel manufacture)
>Nonferrous alloys (improved corrosion resistance and hardness)
>High purity salt for various chemical uses
>Purifying and scavenging agent in metal production
>Manufacture of aluminum by Toth process

>Tables E-54 through E-60 present manganese consumption and emission data.

Storage:
>Protect containers against physical damage. Food and drinks should be kept out of work area.

Transportation:
>Shipped in drums and in car lots in pure, electrolytic, or powdered grades

Disposition:
>Manganese may be disposed of by sanitary landfill.

Sampling and Analytical Methods

1. NIOSH Method 173
    a. Filter collection.
    b. Acid digestion.
    c. AAS (atomic absorption spectrophotometry).

    Detection limit:
    >0.2 mg/m^3 with a 3-liter sample

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TABLE E-54. UNITED STATES MANGANESE ORE CONSUMPTION

Use	Usage, %	Manganese ore consumed, tons/yr
Manganese alloys/metals	79	1,263,581
Pig iron and steel	9	143,761
Dry cells, chemicals, misc.	12	193,581
Total	100	1,600,923

Source: Systems Applications, Inc. 1980.

TABLE E-55. 1978 NATIONWIDE MANGANESE EMISSIONS

Source	Nationwide emissions, lb/yr
Mining	Negligible
Iron and steel	9,212,000
Gray iron foundry	5,540,000
Ferro alloy, ferro manganese, silico manganese	12,632,000
Chemical applications	644,000
Battery production	276,000
Welding rod manufacture	48,000
Power plants	
Coal	5,280,000
Oil	13,566
Industrial Boilers	
Coal	352,000
Oil	14,091
Residential/commercial	
Coal	16,000
Oil	4,454
Coke ovens	1,950,000
Total	35,982,111

Source: Systems Applications, Inc. 1980.

TABLE E-56. MANGANESE EMISSIONS FROM IRON AND STEEL PRODUCTION

Region	Number of sites	Manganese emissions, lb/yr	Average emissions per site	
			lb/yr	g/s
New England	10	55,045	5,505	0.079
Middle Atlantic	65	2,846,685	43,795	0.630
East North Central	84	3,859,795	45,950	0.661
West North Central	5	101,260	20,250	0.292
South Atlantic	22	819,940	37,270	0.537
East South Central	25	626,250	25,050	0.361
West South Central	12	211,865	17,655	0.254
Mountain	2	221,210	110,605	1.592
Pacific	32	469,950	14,685	0.211
Total	257	9,212,000	35,844	

Source: Systems Applications, Inc. 1980.

TABLE E-57. MANGANESE EMISSIONS FROM GRAY IRON FOUNDRY OPERATIONS

Region	Number of sites	Manganese emissions, lb/yr	Average emissions per site	
			lb/yr	g/s
New England	13	138,500	10,655	0.15
Middle Atlantic	42	508,985	12,120	0.17
East North Central	129	2,887,725	22,385	0.32
West North Central	29	315,085	10,865	0.16
South Atlantic	22	408,575	18,570	0.27
East South Central	37	654,410	17,685	0.25
West South Central	19	277,000	14,580	0.21
Mountain	5	65,785	13,157	0.19
Pacific	28	283,925	10,140	0.15
Total	324	5,540,000	17,100	

Source: Systems Applications, Inc. 1980.

TABLE E-58. MANGANESE EMISSIONS FROM FERROALLOY, FERRO MANGANESE, AND SILICA MANGANESE PRODUCTION

Region	Number of sites	Manganese emissions, lb/yr
New England	0	0
Middle Atlantic	12	2,972,220
East North Central	8	1,981,480
West North Central	1	247,685
South Atlantic	8	1,981,480
East South Central	13	3,219,905
West South Central	1	247,685
Mountain	4	990,740
Pacific	4	990,740
Total	51	12,632,000

Source: Systems Applications, Inc. 1980.

TABLE E-59.   MANGANESE EMISSIONS FROM ELECTRICAL UTILITY POWER PLANTS
(coal-fired)

Region	Number of sites	Manganese emissions, lb/yr	Average emissions per site	
			lb/yr	g/s
New England	9	36,960	4,105	0.06
Middle Atlantic	51	596,640	11,700	0.17
East North Central	156	1,789,920	11,475	0.17
West North Central	111	496,320	4,470	0.07
South Atlantic	61	1,034,880	16,965	0.25
East South Central	44	860,640	19,560	0.29
West South Central	3	68,640	22,880	0.33
Mountain	38	359,040	9,450	0.14
Pacific	1	36,960	36,960	0.54
Total	474	5,280,000	11,140	

Source: Systems Applications, Inc. 1980.

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TABLE E-60. MANGANESE EMISSIONS FROM COKE OVEN OPERATIONS

Region	Number of sites	Manganese emissions, lb/yr
New England	0	0
Middle Atlantic	15	479,505
East North Central	25	799,185
West North Central	3	95,900
South Atlantic	4	127,870
East South Central	9	287,705
West South Central	2	63,935
Mountain	2	63,935
Pacific	1	31,965
Total	61	1,950,000

Source: Systems Applications, Inc. 1980.

Possible interferences:
Spectral interferences; background or nonspecific absorption; ionization interferences, chemical interferences; and physical interferences.

2. NIOSH Method 351
   a. Filter collection.
   b. Acid digestion.
   c. Inductively coupled plasma-atomic emission spectroscopy analysis.

Detection limit:
5 to 2000 $\mu g/m^3$ with a 5-liter sample.

Possible interferences:
Physical interferences; chemical interferences; spectral interferences.

3. NIOSH Method S5
   a. Filter collection.
   b. Acid digestion.
   c. Atomic absorption.

Detection limit:
0.2 to 20 mg/m^3 with a 22.5-liter sample.

Possible interferences:
No known interferences.

Permissible Exposure Limits

	OSHA	ACGIH
TWA		1 mg/m^3 (fume)
STEL		3 mg/m^3 (fume)
Ceiling	5 mg/m^3	5 mg/m^3 (dust and compounds)

Human Toxicity

Acute Toxicity:
Occurs by inhalation of the dust or fumes. Symptoms are languor, sleepiness, weakness, emotional disturbances, spastic gait, and paralysis.

Chronic Toxicity:
Chronic manganese poisoning is a clearly characterized disease that results from the inhalation of fumes or dusts of manganese. Exposure to heavy concentrations for as little as three months may produce the condition, but it usually develops after 1 to 3 years of exposure. The central nervous system is the chief site of damage. Manganese has also been found to be an equivocal tumorigenic agent in rats.

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Chemical Name

Mercury

CAS Number

7439-97-6

Chemical Classification

Metallic element

Synonyms

Colloidal mercury; kwik; mercure; mercurio; mercury-metallic (DOT); metallic mercury; NCI-C60399; quecksilber; quicksilver; RTEC

Physical/Chemical Properties

Description:
Silvery, extremely heavy liquid, sometimes found native.

Boiling Point:
356.6°C

Melting Point:
-38.85°C

Molecular Weight:
200.6

Chemical Formula:
Hg

Vapor Pressure:
1 mm at 126.2°C; 2×10^{-3} mm at 25°C

Density:
13.54 g/ml (20°C)

Refractive Index:
Not available

Solubility:
Insoluble in HCl; soluble in sulfuric acid upon boiling; readily soluble in nitric acid; insoluble in water, alcohol, and ether; soluble in lipids.

Log Partition Coefficient (octanol/water):
Not available

Photochemical Reactivity:
    Not photochemically reactive

Chemical Reactivity:
    Incompatible with acetylenic compounds, ammonia, boron diiodo-
    phosphide, ethylene oxide, metals, methyl azide, methylsilane,
    oxygen, oxidants, and tetracarbonylnickel.

Environmental Fate

Breakdown of atmospheric dimethyl mercury is of slight importance.
Oxidation of metallic mercury forms ionic mercury; reduction forms
an HgS precipitate. Metallic Hg, methylated Hg, and adsorbed Hg
all volatilize. Mercury is adsorbed by most particles, buried in
sediment, and reduced to HgS. It is bioaccumulated by all orga-
nisms and readily methylated metabolically.

Source of Emissions

Production:
    By heating cinnabar in air, or with lime, and condensing the
    vapor. Purified by distillation. In 1982 and 1983, Nevada
    was the only mercury-producing State. Producers were the
    Carlin gold mine, the Pinson gold mine, and the McDermitt
    mercury mine. During 1983, four companies specialized in
    processing primary or scrap mercury: Bethlehem Apparatus Co.,
    Hellertown, PA; D.F. Goldsmith Chemical & Metal Corp.,
    Evanston, IL; Mercury Refining Co., Inc., Albany, NY; and Troy
    Chemical Corp., Newark, NJ.

Uses:
    Manufacturing of all mercury salts
    Mercury cells
    Electric switches
    Propellant
    Mercury vapor lamps
    Barometers
    Thermometers
    Medicine
    Amalgams
    Mercury boilers

    Tables E-61 and E-62 present mercury production and consump-
    tion data.

Storage:
    Containers should be kept closed. Preferably, small quanti-
    ties should be stored in a polyethylene bottle, and the mercu-
    ry surface should be covered with water to prevent evaporation
    as much as possible.

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TABLE E-61. MERCURY PRODUCTION
(flasks)

	1979	1980	1981	1982	1983
Producing mines	3	4	3	3	3
Mine production	29,519	30,657	27,904	25,760	25,070
Secondary production					
Industry	4,287	6,793	4,244	4,473	13,474
Government	11,300	10,013	7,000	-	-
Industry stocks, year end	27,582	33,069	27,339	29,327	31,518
Shipments from the National Defense Stockpile	196	-	-	7,088	6,000
Imports for consumption	26,448	9,416	12,408	8,916	12,786
Consumption, reported	62,205	58,983	59,244	48,943	49,138
Consumption, apparent	82,721	51,392	57,286	44,249	55,252

Source: Minerals Yearbook.

TABLE E-62. MERCURY CONSUMED IN THE UNITED STATES, BY USE
(flasks)

SIC code	Use	1979	1980	1981	1982	1983
28	Chemical and allied products:					
2812	Chlorine and caustic soda manufacture	12,180	9,470	7,323	6,243	8,054
2816	Pigments	W[a]	W	W	W	W
2819	Catalysts, miscellaneous	1,257	765	815	499	484
2821	Catalysts for plastics	W	W	W	W	W
2819	Laboratory uses	410	363	328	281	280
2851	Paints	9,979	8,621	7,049	6,794	6,047
2879	Agricultural chemicals	W	W	79	36	W
-	Other chemicals and allied products	82	W	W	W	W
36	Electrical and electronic uses:					
3641	Electric lighting	511	1,036	1,043	826	1,273
3643	Wiring devices and switches	3,213	3,062	2,641	2,004	2,316
3692	Batteries	25,299	27,829	29,441	24,880	23,350
-	Other electrical and electronic uses	106	144	W	W	W
38	Instruments and related products:					
382	Measuring and control instruments	3,603	3,049	5,671	3,064	2,465
3843	Dental equipment and supplies	1,422	1,779	1,613	1,019	1,597
-	Other instruments and related products	192	190	253	194	W
-	Other	556	790	242	984	1,356
	Total	62,205	58,983	59,244	48,943	49,138

[a] W = Withheld to avoid disclosing company proprietary data; included in "Total".

Source: Minerals Yearbook.

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Transportation:
Transported in 1-, 5-, and 10-pound bottles and 76-pound flasks.

Disposition:
Elemental mercury may be accumulated for sale or for purification and reuse. Inorganic mercury (mercuric chloride, mercuric nitrate, mercuric sulfate) may be disposed of by incineration followed by recovery/removal of mercury from the gas stream. Alternatively, mercury compounds may be recovered from brines, sludges, and spent catalysts. Mercury in inaccessible locations (cracks, etc.) can be treated with calcium polysulfide and excess sulfur.

Sampling and Analytical Methods

1. NIOSH Method
   a. Solid Sorbent Tube (30 mg silvered chromosorb P, with glass-fiber prefilter.
   b. Automatic absorption, flameless.

   Detection limit:
   0.3 ppb per 3-liter sample

   Possible interferences:
   Chlorine, along with other oxidizing gasess, will attack silver. Methyl mercuric chloride is a potential interferent.

Permissible Exposure Limits

	OSHA	ACGIH (skin)	NIOSH
TWA		0.05 mg/m³ air (all forms except alkyl vapor)	0.05 mg/m³
		0.1 mg/m³ (aryl and inorganic compounds)	
		0.01 mg/m³ (alkyl compounds)	
Ceiling	1 mg/10m³	0.03 mg/m³ (alkyl compounds)	

Human Toxicity

Acute Toxicity:
Gastrointestinal tract effects, central nervous system effects. High toxicity inhalation. A general protoplasmic poison after absorption, it circulates in the blood and is stored in the liver, kidneys, spleen, and bone. Solution salts have violent corrosive effects on skin and mucous membranes, severe nausea, vomiting, abdominal pain, bloody diarrhea, kidney damage; death usually occurs within 10 days.

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Chronic Toxicity:
 Mercury has a cumulative effect and has a tendency to deposit
 in certain organs; most notably the brain, liver, and kidneys,
 although it can be found in nearly all tissues. The TLV is
 set at a point to prevent chronic poisoning. The onset of
 symptoms of mercury toxicity from chronic exposure may be
 ignored by the individual or attributed to other causes. This
 is particularly true with erethism, which is characterized by
 irritability, outbursts of temper, excitability, shyness,
 resentment of criticism, headache, fatigue, and indecision.

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Chemical Name

Methylene chloride

CAS Number

75-09-2

Chemical Classification

Chlorinated hydrocarbon

Synonyms

Aerothene MM; chlorure de methylene; DCM; dichloromethane; dichloromethane (DOT); freon 30; methane dichloride; methylene bichloride; methylne chloride; methylene chloride (DOT); methylene dichloride; metylenu chlorek; narkotil; NCI-C50102; solaesthin; solmethine

Physical/Chemical Properties

Description:
Colorless volatile liquid; penetrating ether-like odor.

Boiling Point:
40.1°C

Melting Point:
-97°C

Molecular Weight:
84.9

Chemical Formula:
CH_2Cl_2

Vapor Pressure:
380 mm at 22°C

Vapor Density:
2.93 (air = 1)

Refractive Index:
$N_D^{20} = 1.4242$

Solubility:
Soluble in alcohol and ether; slightly soluble in water.

Log Partition Coefficient (octanol/water):
1.25

Photochemical Reactivity:
    Reactivity toward OH· is a half-life of approximately 1 year,
    less than methane. No reaction toward O_3.

Chemical Reactivity:
    When heated to decomposition, emits highly toxic fumes of
    phosgene. Not explosive under ordinary conditions, but will
    form explosive mixtures in atmosphere having high oxygen
    content or in liquid O_2, N_2O_4, K, Na, NaK. Reacts violently
    with Li, NaK, potassium-tert-butoxide, and (KOH+n-methyl-n-
    nitrosourea).

Environmental Fate

    Because of high vapor pressure, volatilization to the atmosphere is
    rapid and is a major transport process. In tetrosphere, oxidation
    by hydroxyl radicals to carbon dioxide, carbon monoxide, and phos-
    gene is important fate mechanism.

Source of Emissions

Production/processing:
    Chlorination of methyl chloride and subsequent distillation.
    Chlorination of methane and subsequent distillation.

Uses:

Aerosol products	Solvent for triacetate extrusion
Paint removers	Solvent in the pharmaceutical and
Solvent degreasing	electronics industry
Plastics processing	Photographic film
Blowing agent in foams	Polycarbonate resins
Solvent in inks, adhesives	Cleaning uses

    Tables E-63 through E-67 present methylene chloride produc-
    tion, consumption, and emission data.

Storage:
    Should be protected against physical damage and stored in a
    cool, dry, well-ventilated location, away from any area where
    the fire hazard may be acute.

Transport:
    Should be shipped in glass bottles, 5- and 55-gallon drums,
    tank cars, and tank trucks.

Disposition:
    Methylene chloride may be disposed of by incineration after
    mixing with another combustible fuel; care must be exercised
    to assure complete combustion to prevent the formation of
    phosgene. An acid scrubber is necessary to remove the halo
    acids produced.

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TABLE E-63. PRODUCTION OF METHYLENE CHLORIDE

Company	Location	1978 estimated production,[a] 10^6 lb/yr	Process[b]	1978 estimated capacity, 10^6 lb/yr	Geographical location, latitude/longitude
Allied Chemical Corp.	Moundsville, WV	31	A,B[c]	50	39 54 24/80 47 51
Diamond Shamrock	Belle, WV	63	A	100	38 14 09/81 32 38
Dow Chemical	Freeport, TX	125	B	200	28 59 15/95 24 45
	Plaquemine, LA	112	A	180	30 19 00/91 15 00
Stauffer	Louisville, KY	38	A	60	38 12 09/85 51 49
Vulcan Materials Co.	Geismar, LA	50	A	80	30 10 00/90 59 00
	Wichita, KS	106	A,B[d]	170	37 36 55/97 18 30
Total		525		840	

[a] Distribution of the 525 million pounds per year for each producing location has been made as a direct ratio of total production/total capacity x individual plant capacity.

[b] (A) - Methanol hydrochlorination process or methyl chloride chlorination process.
(B) - Methane chlorination process.

[c] 5% methane chlorination, 95% methyl chloride chlorination.

[d] 10% methane chlorination, 90% methyl chloride chlorination.

Source: Systems Applications, Inc. 1980.

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TABLE E-64. 1978 METHYLENE CHLORIDE CONSUMPTION BY END USE

End use	Percent of total consumption	End use consumption, 10^6 lb/yr
Paint and varnish remover	30	157.5
Metal degreasing	22	115.5
Aerosols	17	89.25
Plastics processing	5	26.25
Export	21	110.25
Miscellaneous	5	26.25
Total	100	525

Source: Systems Applications, Inc. 1980.

TABLE E-65. 1978 METHYLENE CHLORIDE NATIONWIDE EMISSION LOSSES

End use	Estimated national emission, 10^6 lb/yr
Production	0.65
Paint and varnish remover	157.5
Metal degreasing	107.1
Aerosols	89.25
Plastics processing	26.25
Miscellaneous	26.25
Export	0
Total	407.00

Source: Systems Applications, Inc. 1982.

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TABLE E-66. 1978 METHYLENE CHLORIDE PRODUCTION EMISSIONS

Company	Location	Process vent emissions		Storage vent emissions		Fugitive emissions		Total emissions	
		lb/yr	g/s	lb/yr	g/s	lb/yr	g/s	lb/yr	g/s
Allied Chemical	Moundsville, WV	980	0.014	74,030	1.066	14,430	0.208	89,440	1.288
Diamond Shamrock	Belle, WV	164	0.002	15,498	0.223	2,980	0.043	18,642	0.268
Dow Chemical	Freeport, TX	16,353	0.235	119,566	1.720	37,780	0.543	173,699	2.498
	Plaquemine, LA	234	0.003	22,178	0.319	4,268	0.061	26,680	0.383
Stauffer	Louisville, KY	990	0.014	93,480	1.346	17,970	0.259	112,440	1.619
Vulcan	Geismar, LA	1,300	0.019	123,000	1.771	23,650	0.340	147,950	2.130
	Wichita, KA	3,960	0.057	24,553	0.353	48,550	0.699	77,063	1.109
Total		23,981		472,305		149,628		645,914	

Source: Systems Applications, Inc. 1980.

TABLE E-67. EMISSIONS RATES AND NUMBER OF GENERAL POINT SOURCES OF METHYLENE CHLORIDE

Region	Cold cleaning		Open-top vapor degreasing		Conveyorized vapor degreasing	
	Emissions/site, gm/s	Number of sites	Emissions/site, gm/s	Number of sites	Emissions/site, gm/s	Number of sites
New England	0.00952	7,284	0.288	82	0.857	14
Middle Atlantic	0.00952	18,892	0.288	170	0.857	30
East North Central	0.00952	32,084	0.288	257	0.857	50
West North Central	0.00952	10,624	0.288	66	0.857	10
South Atlantic	0.00952	14,620	0.288	69	0.857	10
East South Central	0.00952	7,168	0.288	39	0.857	6
West South Central	0.00952	11,764	0.288	59	0.857	8
Mountain	0.00952	4,397	0.288	26	0.857	3
Pacific	0.00952	14,347	0.288	132	0.857	20

Source: Systems Applications, Inc. 1980.

Sampling and Analytical Methods

1. NIOSH Method S329
   a. Adsorption on charcoal.
   b. Desorption with carbon disulfide.
   c. Gas chromatography.

   Detection limit:
   350 to 10,400 mg/m^3 (100-3000 ppm) per 1-liter sample

   Possible interferences:
   High humidity will lower vapor trapping efficiency. Any compound with the same retention time as methylene chloride may be an interferent.

2. NIOSH Method P&CAM 127
   a. Adsorption on charcoal.
   b. Desorption with carbon disulfide.
   c. Gas chromatography.

   Detection limit:
   0.05 mg/sample (0.01 ppm); minimum 0.5-liter sample

   Possible interferences:
   High humidity will lower vapor trapping efficiency. Any compound with the same retention time as methylene chloride may be an interferent.

3. NIOSH Method 1005 (replaces NIOSH Methods S329 and P&CAM 127)
   a. Solid sorbent tube (two coconut shell charcoal tubes; 100 mg/50 mg).
   b. Gas chromatography.
   c. Flame ionization detector.

   Detection limit:
   3.0 ppm per 1-liter sample

   Possible interferences:
   None identified.

4. Method B (Appendix A) C_2-C_{18} hydrocarbons and other nonpolar organics with a boiling point of 100° to 175°C.
   a. Whole air collection in canister.
   b. Cryogenic concentration.
   c. Gas chromatography/flame ionization detection.

   Detection limit:
   0.1 ppb per 100-ml sample

   Possible interferences:
   Storage times greater than a week are not recommended. Laboratory contamination with methylene chloride is a common problem.

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5. Method F (Appendix A) nonpolar volatiles with a boiling point 0° to 100°C.
   a. Adsorption on carbon molecular sieves.
   b. Thermal desorption into canister.
   c. Analysis by gas chromatography/flame ionization detection or gas chromatography/mass spectrometry analysis.

Detection limit:
   0.01-1 ppb per 20-liter sample

Possible interferences:
   High temperature (350°C) required for desorption may decompose compounds. Laboratory contamination with methylene chloride is a common problem.

Permissible Exposure Limits

	OSHA	ACGIH
TWA	500 ppm	100 ppm (350 mg/m^3)
STEL		500 ppm (1740 mg/m^3)
Ceiling	1000 ppm	
Peak	2000 ppm (5 min. in 2 h)	

The ACGIH has listed methylene chloride for intended changes to delete the STEL.

Odor perception 25 to 50 ppm.

Human Toxicity

Acute toxicity:
   Very dangerous to the eyes. Except for its property of inducing narcosis, it has very few other acute toxicity effects. Can be decomposed by contact with hot surfaces or open flame, which yields toxic fumes that are irritating. Can cause dermatitis upon prolonged skin contact.

Chronic Toxicity:
   EPA is awaiting the results of a National Toxicology Program peer review of a methylene chloride bioassay (February 1985). Preliminary findings of the bioassay are that methylene chloride is carcinogenic to laboratory animals.

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Chemical Name

4,4-Methylenedianiline

CAS Number

101-77-9

Chemical Classification

Aromatic Amine

Synonyms

4-(4-aminobenzyl) aniline; bis-p-aminofenylmethan; bis(p-aminophenyl) methane; bis(4-aminophenyl) methan; DADPM; DAPM; DDM; P,P'-diamino-fenylmethan; 4,4'-diaminodiphenylmethan; diaminodiphenylmethane; P,P'-diaminodiphenylmethane; 4,4'-diaminodiphenylmethane; di-(4-aminophenyl) methane; dianalinemethane, dianilinomethane, 4,4'-diphenylmethanediamire; EPICURE DDM; HT 972; MDA; methylenebis (aniline); 4,4'-methylenebisaniline; methylenedianiline; p,p'-methylenedianiline; 4,4'-methylenedianiline; TONOX.

Physical/Chemical Properties

Description:
Crystals from water or benzene; tan flakes or lumps, faint amine-like odor.

Boiling Point:
398° to 399°C

Melting Point:
92° to 93°C

Molecular Weight:
198.3

Chemical Formula:
$H_2NC_6H_4CH_2C_6H_4NH_2$

Vapor Pressure:
Negligible (0.2 mm Hg for one form)

Density:
1.056 g/m³ (liquid at 100°C)

Refractive Index:
Not available

Solubility:
Slightly soluble in cold water. Very soluble in alcohol, benzene, ether.

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Log Partition Coefficient (octanol/water):
Estimated between 1.8 and 2.5

Photochemical Reactivity:
No primary information is available, but the known photochemical reactivity of both toluene and aniline suggests that MDA may also be reactive.

Chemical Reactivity:
Weak base; has the general characteristics of primary aromatic amines. Most reactions involve substitution of the amine hydrogens or aromatic hydrogens. In some cases, the functional groups are totally altered. Polymers are formed when the amine is condensed with multifunctional reactants. Decomposes to highly toxic fumes of aniline and NO_x.

Environmental Fate

Only limited information is available on the chemical and biological transformation of MDA in the environment. MDA appears to undergo reactions typical of both aromatic amines and aromatic compounds in general. The low vapor pressure of MDA crystals make it improbable that MDA molecules evaporate readily to the atmosphere. No information was found to indicate bioaccumulation of MDA.

Source of Emissions

Production:
Acid catalyzed reaction of aniline with formaldehyde.

Uses:
Ninety-nine percent is consumed to manufacture methylene phenyl diisocyanate (MDI).

Other uses include epoxy and urethane curing, production of ketamines, wire coatings, circuit board coatings, dye intermediates, rubber processing chemicals, pharmaceuticals, and herbicides.

Tables E-68 and E-69 present MDA production and consumption data.

Storage:
Sold as a viscous liquid or lump in the crude form or as flakes or granules in the pure form. Stored in tanks, 55-gallon drums, bags, or kegs. Generally, containers consist of fibrous material.

TABLE E-68. PRESENT AND PROPOSED MDA MANUFACTURING PLANTS

Company	Plant location	Comments
BASF Wyandotte Corp.	Parsippany, NJ Geismar, LA	Presently imports MDA. Had a 1977 capacity of less than 100,000 pounds/year. New plant scheduled for operation by 1985 with a capacity of 120 million pounds/year.
E.I. du Pont de Nemours	Belle, WV	Between 10 and 15 million pounds of MDA production in 1977. All production used to prepare Du Pont Spandex fibers and Quiana resins. Qiana resins no longer produced using MDA.
Mobay Chemical Corp.	New Martinsville, WV Baytown, TX	All MDA consumed onsite to produce MDI. The 1980 production capacities were 79 million pounds/year at each facility. The Baytown plant is scheduled to double its capacity by 1985.
Olin Corp.	Moundsville, WV (formerly Allied)	Olin does not produce MDI and is the only supplier of pure MDA. The 1972-73 production was approximately 2 million pounds.
Rubicon Chemicals Inc.	Geismar, LA	Most MDA is used to produce MDI. Present MDA capacity is approximately 79 million pounds/year. Expansion is planned to increase MDA capacity to 200 million pounds/year by 1985.
Uniroyal, Inc.	Naugatuck, CT	Polymeric MDA available as Tonox. MDA capacity unknown.
Upjohn Co.	La Porte, TX	Most MDA is used to produce MDI. MDA capacity in 1980 was 213 million pounds/year.

Note: ARCO chemical has a plant scheduled for operation in 1985 to produce MDI by a process that does not use MDA as an intermediate. MDI capacity 150 million pounds/year.

Source: PEI Associates, Inc. 1983.

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TABLE E-69. ESTIMATED CONSUMPTION OF MDA FOR NON-MDI USES

End-use application	Estimated pounds/ year of pure MDA	Estimated pounds/ year of polymeric MDA
Epoxy curing	200,000-450,000	1,500,000
Urethane curing	50,000	a
Ketamine production	40,000	a
Wire coating production	220,000	a
Production of coatings for printed circuit boards and aircraft parts	50,000	a
Dye intermediates	50,000	a
Rubber processing chemical	10,000	b
Corrosion inhibitor	0	a
Antioxidant for lubricating oil	0	200,000
Intermediate for pharmaceuticals, herbicides, etc.	140,000	a

a No information found.

b Although no estimate was reported, it is believed that some polymeric MDA is used for this purpose.

Source: PEI Associates, Inc. 1983.

Transportation:
 Shipped in bulk by tank car or in packaged container by truck.
 No special handling procedures.

Disposition:
 Ninety-nine plus percent is consumed in chemical reactions.
 Any unreacted or spilled material is probably disposed of in a
 sanitary landfill.

Sampling and Analytical Methods

Limited information regarding sampling and analytical methods for
MDA was reported by JRB Associates (1981). Adsorption onto activa-
ted charcoal, XAD-2, and XAD-4 was reported for aqueous solutions.
No references were found for vapor monitoring of MDA. Analyses by
liquid chromatography, visible spectrometry, and wet chemical
methods have been reported. No data on any monitoring of MDA in
the environment could be found.

Permissible Exposure Limits

	OSHA	ACGIH (skin)
TWA	Not established	0.1 ppm (0.8 mg/m^3)
STEL		0.5 ppm (4 mg/m^3)

The ACGIH has listed MDA for intended changes to delete the STEL
and add notation that MDA is an industrial substance suspected of
carcinogenic potential in man.

Human Toxicity

Acute Toxicity:
 An eye irritant. Human systemic effects. High toxicity via
 oral, subcutaneous, and intraperitoneal routes. Does not seem
 to be readily absorbed through the skin.

Chronic Toxicity:
 MDA has been shown to be carcinogenic in both sexes of rats
 and mice in bioassays conducted by the National Toxicology
 Program and is considered a potential carcinogen in humans.

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Chemical Name

Perchloroethylene

CAS Number

127-18-4

Chemical Classification

Chlorinated hydrocarbon (unsaturated)

Synonyms

Ankilostin; antisol 1; carbon bichloride; carbon dichloride; czterochloroetylen; didakene; dow-per; ENT-1860; ethene, tetrachloro-; ethylene tetrachloride; fedal-UN; NCI-C04580; NEMA; PER; perawin; PERC; perchloerethyleen, per; perchloroethylene; perclene; percloroetilene; percosolve; perk; perklore; persec; tetlen; teracap; tetrachlooretheen; tetrachloraethen; tetrachlorethylene; tetrachloroethene; tetrachloroethylene; 1,1,2,2-tetrachloroethylene; tetrachloroethylene (DOT); tetracloroefeen; tetraleno; tetralex; tetravec; tetrogner; tetropil.

Physical/Chemical Properties

Description:
Colorless liquid; ether-like odor

Boiling Point:
121°C

Melting Point:
-22.4°C

Molecular Weight:
165.8

Chemical Formula:
$Cl_2C:CCl_2$

Vapor Pressure:
15.8 mm at 22°C

Vapor Density:
5.83 (air = 1)

Refractive Index:
$N_D^{25} = 1.5029$

Solubility:
Miscible with alcohol, ether, and oils in all proportions; insoluble in water.

Log Partition Coefficient (octanol/water):
   2.88

Photochemical Reactivity:
   Photochemically reactive

Chemical Reactivity:
   When heated to decomposition, emits toxic chloride fumes.
   Material is extremely stable and resists hydrolyzers. Reacts
   violently with Ba, Be, Li, N_2O_4, and NaOH. May be handled in
   the presence or absence of air, water, and light with any of
   the common construction materials at a temperature up to
   140°C.

Environmental Fate

   The predominant fate of perchloroethylene is tropospheric photo-
   oxidation by hydroxyl radicals, which yields trichloroacetyl-chlo-
   ride and phosgene. Rapid volatilization is the primary transport
   process. There is a moderate potential for bioaccumulation and
   possible biodegradation by higher organisms.

Source of Emissions

Production:
   Made by chlorination of hydrocarbons, and pyrolysis of the
   carbon tetrachloride also formed.
   From acetylene and chloride via trichloroethylene.

Uses:
   Dry cleaning solvent
   Manufacture of fluorocarbons
   Vapor-degreasing solvent
   Drying agent for metals and certain other solids
   Textile processing
   Vermifuge
   Heat transfer medium

   Tables E-70 through E-74 present perchloroethylene production,
   consumption, and emission data.

Storage:
   Store in a cool, dry, well-ventilated location, away from any
   area where the fire hazard may be acute.

Transportation:
   Shipped in 5- and 55-gallon steel drums, tank cars, and tank
   trucks.

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TABLE E-70. LOCATIONS OF AND PRODUCTION FIGURES FOR
PERCHLOROETHYLENE FACILITIES

Location	Company[a]	Manufacturing process[b]	1978 capacity, 10^6 kg	1978 estimated production, 10^6 kg
California Pittsburg	Dow Chemical USA	Cl-HC	20	10
Kansas Wichita	Vulcan Materials Co.	Cl-HC	20	10
Kentucky Louisville	Stauffer Chemical Co.	Cl-HC	30	20

Louisiana
  Baton Rouge
  Geismar
  Lake Charles
  Plaquemine
	Ethyl Corporation
	Vulcan Materials Co.
	PPG Industries, Inc.
	Dow Chemical
		Cl-EDC
		Cl-HC
		Ox-EDC
		Cl-HC
			20
			70
			90
			50
				10
				40
				50
				30

Texas
  Corpus Christi
  Deer Park
  Freeport
	DuPont[c]
	Diamond Shamrock
	Dow Chemical
		Cl-HC
		Cl-EDC
		Cl-EDC
			70
			75
			70
				40
				40
				40

Total			515	290

[a]An August 1978 article in Chemical Marketing Reporter stated that the Hooker Chemical Corporation facility at Taft, Louisiana stopped producing perc in March 1978.

[b]Key to symbols: Cl-HC = Chlorination of C_1 to C_3 hydrocarbons or their partially chlorinated derivatives; Cl-EDC = chlorination of ethylene dichloride; Ox-EDC = oxychlorination of ethylene dichloride.

[c]Captive use only.

SRI International, 1979.

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TABLE E-71. ESTIMATED CONSUMPTION OF PERCHLOROETHYLENE BY TYPE OF USE
1978

Type of use	Consumption, 10^6 kg	Percent of total
Dry cleaning	160	53
Metal cleaning	50	17
Chemical intermediate	40	13
Textile processing	20	7
Miscellaneous	30	10
Total	300	100

Source: SRI International, 1979.

TABLE E-72. ESTIMATED NUMBER OF URBAN DRY CLEANERS USING
PERCHLOROETHYLENE BY SIZE OF OPERATION

Type of operation	Number of operations			By number of employees		Total
	1 to 4	5 to 9	10 to 19	20 to 49	>50	
Commercial	4,200	1,900	850	700	120	7,770
Coin-operated	3,700	500	120	60	10	4,390
Industrial	20	10	20	100	110	260

Source: SRI International, 1979.

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TABLE E-73. ESTIMATED PERCHLOROETHYLENE USED FOR DEGREASING
IN THE MANUFACTURING INDUSTRY

SIC Code[a]	Fraction using perchloroethylene Number of employees		Amount of perchloroethylene used per plant, gal/year Number of employees		
	0 to 20	>20	0 to 20	20 to 100	>100
331	0.00	0.11	-	1,800[a]	10,000
336	0.00	0.06	-	45[a]	250
339	0.00	0.14	-	12,000	67,200[a]
342	0.00	0.09	-	2,655[a]	14,752
343	0.00	0.14	-	2,750	15,400[a]
344	0.00	0.08	-	350	1,960[a]
345	0.00	0.18	-	863[a]	4,795
347	0.08	0.11	330	5,262	17,044[a]
349	0.00	0.14	-	1,310	7,336[a]
352	0.00	0.11	-	90[a]	500
361	0.00	0.07	-	149[a]	825
362	0.17	0.00	219	-	-
364	0.00	0.07	-	73[a]	403
366	0.00	0.11	-	176[a]	980
367	0.06	0.00	700	-	-
371	0.00	0.05	-	110	616[a]
372	0.10	0.22	10	490	25,703

[a]These amounts have been extrapolated on the basis of the number of employees in the plant.

Source: SRI International, 1979.

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TABLE E-74. ESTIMATED EMISSIONS FROM PERCHLOROETHYLENE FACILITIES

Location	Company	Estimated annual emissions 10^3 kg	Estimated emission rate g/s
California Pittsburg	Dow Chemical USA	20	0.63
Kansas Wichita	Vulcan Materials Co.	20	0.63
Kentucky Louisville	Stauffer Chemical Co.	40	1.27
Louisiana			
Baton Rouge	Ethyl Corporation	20	0.63
Geismar	Vulcan Materials Co.	80	2.54
Lake Charles	PPG Industries, Inc.	250	7.90
Plaquemine	Dow Chemical	60	1.90
Texas			
Corpus Christi	DuPont[a]	80	2.54
Deer Park	Diamond Shamrock	80	2.54
Freeport	Dow Chemical	80	2.54

[a]Captive use for C_2 fluorocarbons; emission factor is unchanged.

Source: SRI International, 1979.

Disposition:
    Perchloroethylene may be disposed of by incineration, prefer-
    ably after mixing with another combustible fuel. Care must be
    exercised to assure complete combustion to prevent the forma-
    tion of phosgene. An acid scrubber is required to remove the
    halo acids produced. Alternatively, perchloroethylene may be
    recovered from waste gases and reused.

Sampling and Analytical Methods

1. NIOSH Method S335
    a. Adsorption on charcoal.
    b. Desorption with carbon disulfide.
    c. Gas chromatography.

    Detection limit:
        136 to 4065 ng/m³ (20 to 600 ppm) for 3-liter sample

    Possible interferences:
        High humidity will lower vapor trapping efficiency. Any
        compound with the same retention time as perchloroethylene
        may be an interferent.

2. NIOSH Method P&CAM 127
    a. Adsorption on charcoal.
    b. Desorption with carbon disulfide.
    c. Gas chromatography.

    Detection limit:
        0.6 mg/m³ (0.01 ppm) with a 1-liter minimum sample size

    Possible interferences:
        High humidity will lower vapor trapping efficiency. Any
        compound with the same retention time as perchloroethylene
        may be an interferent.

3. Method B (Appendix A): C_2-C_{18} hydrocarbons and other nonpolar
    organics with a boiling point - 100° to 175°C.
    a. Whole air collection in canister.
    b. Cryogenic concentration.
    c. Gas chromatography/flame ionization detection (gas
        chromatography/electron capture detection may also be
        used).

    Detection limit:
        0.1 ppb per 100-ml sample

    Possible interferences:
        Storage time greater than a week is not recommended.

4. Method C (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with a boiling point between 60° and 200°C.
   a. Adsorption on Tenax.
   b. Thermal desorption.
   c. Gas chromatography/mass spectrometry analysis (gas chromatography/electron capture detection may also be used).

   Detection limit:
       1 to 200 ppt for a 20-liter sample

   Possible interferences:
       Blank levels usually limit sensitivity artifacts due to reactive components (O_3, NO_x). Sample can be analyzed only once.

5. Method D (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with a boiling point of 60° to 200°C.
   a. Adsorption on Tenax.
   b. Thermal desorption into canisters.
   c. Gas chromatography/flame ionization detection, or gas chromatography/mass spectrometry analysis (gas chromatography/electron capture detection may also be used).

   Detection limit:
       0.01 to 1 ppb for a 20-liter sample

   Possible interferences:
       Blanks and artifact problems in Method C, above.

Permissible Exposure Limits

	OSHA	ACGIH
TWA	100 ppm	50 ppm (335 mg/m^3)
STEL		200 ppm (1,340 mg/m^2)
Ceiling	200 ppm	
Peak	300 ppm (5 min. in 3 h)	

Human Toxicity

Acute Toxicity:
    Moderate irritation effects via inhalation, oral, subcutaneous, intraperitoneal, and dermal routes. High toxicity via intravenous route. Not corrosive or dangerously acutely reactive, but toxic by inhalation, by prolonged or repeated contact with skin or mucous membrane, or when ingested by mouth. The liquid can cause injuries to the eyes. Exposures to higher than 200 ppm causes irritation, lachrymation, burning of the eyes, and irritation of the nose and throat. There may be vomiting, nausea, drowsiness, an attitude of

irresponsibility, and even the appearance of alcholic intoxication. Also acts as an anesthetic. Can cause dermatitis, particularly after repeated or prolonged contact with skin, preceded by reddening and burning and more rarely, a blistering of the skin.

Chronic Toxicity:
Perchloroethylene caused hepatocellular carcinomas in mice of both sexes; however, a carcinogenesis bioassay was negative in rats. Therefore, perchloroethylene can be considered a suspected animal carcinogen.

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Chemical Name

Phenol

CAS Number

108-95-2

Chemical Classification

Phenol (aromatic alcohol)

Synonyms

Acide carbolique; Bakers P and S liquid and ointment; carbolic acid; carbolic acid (DOT); carbolsaure; fenol; fenolo; hydroxy-benzene; monohydroxybenzene, NCI-50124; oxybenzene; phenic acid; phenole; phenyl hydrate; phenyl hydroxide; phenylic acid; phenylic alcohol.

Physical/Chemical Properties

Description:
White crystalline mass that turns pink or red if not perfectly pure or if under influence of light; absorbs water from the air and liquifies; distinctive odor; sharp burning taste. When in very weak solution, has a sweetish taste.

Boiling Point:
182°C

Melting Point:
42.5° to 43°C

Molecular Weight:
94.1

Chemical Formula:
C_6H_5OH

Vapor Pressure:
1 mm at 40.1°C

Vapor Density:
3.24 (air = 1)

Refractive Index:
$N_D^{41} = 1.5408$

Solubility:
    Soluble in alcohol, water, ether, chloroform, glycerol, carbon
    disulfide, petrolatum, fixator volatile oils or alkalines.

Log Partition Coefficient (octanol/water):
    1.46

Photochemical Reactivity:
    Reactivity toward OH· is 2 times butane. Reactivity toward O_3
    is a 9.6-hour half-life or 15 percent of propylene.

Chemical Reactivity:
    Reacts violently with ($AlCl_3$ + nitrobenzene), butadiene,
    peroxydisulfuric acid, and peroxymonosulfuric acid. Moderate
    fire hazard when exposed to heat, flame, or oxidizers. When
    heated, emits toxic fumes, can react with oxidizing materials.

Environmental Fate

    Photooxidation of volatilized phenol and photolysis of phenolic
    anion may both take place at moderate rates. Metal catalyzed
    oxidation may take place in highly aerated waters. No bioaccumu-
    lation, but extensive biodegradation in natural waters.

Source of Emissions

    Production:
        Oxidation of cumene
        Derivation from benzoic acid

    Uses:
        Phenolic resins
        Epoxy resins (bisphenol-A)
        Nylon 6 (caprolactam)
        2,4-D
        Selective solvent for refining lubricating oils
        Adipic acid
        Salicylic acid
        Phenolphthaline
        Pentachlorophenol
        Acetophenetidine
        Picric acid
        Germicidal paints
        Pharmaceuticals
        Laboratory reagent
        Dyes and indicators
        Slimicide
        General disinfectant

    Tables E-75 through E-83 and Figure E-5 present phenol produc-
    tion, consumption, and emission data.

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TABLE E-75. PHENOL PRODUCERS (NATURAL PHENOL)

Company	Location	1978 capacity,[a] 10^6 lb/yr	1978 production,[a] 10^6 lb/yr	Geographical location, latitude/longitude
Ferro Corporation	Sante Fe Springs, CA	12	5.4	33 56 30/118 04 18
Koppers	Follansbee, WV	12	5.4	40 23 10/80 35 07
Merichem	Houston, TX	12	5.4	29 45 36/95 10 48
Stimson Lumber	Anacortes, WA	12	5.4	48 28 31/122 32 48
U.S. Steel Corporation	Clairton, PA	12	5.4	40 18 15/79 52 43
Total		60	27	

[a] Total capacity and production distributed evenly over all five sites in the absence of capacity figures.

Source: Systems Applications, Inc. 1980.

TABLE E-76. PHENOL PRODUCERS (SYNTHETIC PHENOL)

Company	Location	1978 capacity, 10^6 lb/yr	1978 production,[a] 10^6 lb/yr	Geographical location, latitude/longitude
Allied Chemical	Philadelphia, PA	600	453	40 00 24/75 04 07
Clark	Blue Island, IL	88	66	41 39 21/87 41 56
Dow	Freeport, TX	465	351	28 59 12/95 24 05
Georgia Pacific	Plaquemine, LA	265	200	30 15 00/91 11 00
Getty	El Dorado, KS	95	72	37 47 10/96 52 00
Kalama	Kalama, WA	75	57	46 00 54/122 51 05
Monsanto	Chocolate Bayou, TX	500	377	20 14 55/95 12 45
Shell	Deer Park, TX	500	377	29 42 57/95 07 28
Standard Oil of California	Richmond, CA	55	42	37 56 12/122 20 48
Union Carbide	Bound Brook, NJ	180	135	40 33 32/74 31 18
U.S. Steel	Haverhill, OH	325	245	38 34 52/82 49 36
Total		3148	2375	

[a] Total production distributed based on individual site capacity.

Source: Systems Applications, Inc. 1982.

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TABLE E-77. PHENOL END-USE 1978
(SYNTHETIC AND NATURAL PHENOL)

Source	Usage, 10^6 lb/yr	Percent usage
Phenolic resins	1045	44
Bisphenol-A	405	17
Caprolactam	355	15
Nonylphenol	48	2
Salicylic acid	48	2
Dodecylphenol	24	1
Adipic acid	24	1
Miscellaneous	382	15
Exports	71	3
Total	2402	100

Source: Systems Applications, Inc. 1980.

TABLE E-78. 1978 PHENOL NATIONWIDE EMISSIONS

Source	Nationwide emissions, lb/yr
Production	3,708,080
Phenolic resins	522,500
Bisphenol-A	202,500
Caprolactam[a]	511,200
Nonylphenol	41,700
Salicylic acid	24,000
Dodecylphenol	24,000
Miscellaneous	259,760
Export	0
Total	5,293,740

[a] Includes emissions from adipic acid manufacture.

Source: Systems Applications, Inc. 1982.

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TABLE E-79. PHENOL USER LOCATIONS

Company	Location	1978 capacity, 10^6 lb/yr	1978 production, 10^6 lb/yr	Geographical location, latitude/longitude
	Bisphenol-A producers			
Dow	Freeport, TX	150	95	28 59 12/95 24 05
General Electric	Mount Vernon, IN	220	140	37 56 42/87 34 25
Shell	Deer Park, TX	150	95	29 42 55/95 07 34
U.S. Steel	Haverhill, OH	120	75	38 34 52/82 49 36
	Total	640	405	
	Caprolactam producer			
Allied	Hopewell, VA	400	355	37 22 13/77 18 08
	Total	400	355	
	Nonylphenol producers			
Borg Warner	Morgantown, WV	60	10	39 40 39/80 58 34
Exxon	Bayway, NJ	20	3	40 38 46/74 11 48
GAF	Calvert City, KY	5	1	37 02 50/88 21 12
	Linden, NJ	20	3	40 38 19/74 15 26
Jefferson	Port Neches, TX	35	6	29 57 45/93 56 00
Kalama	Kalama, WA	20	3	46 00 54/122 51 05
Monsanto	Kearney, NJ	40	6	40 46 12/74 09 08
Rohm and Haas	Deer Park, TX	10	2	29 43 30/95 06 15
	Philadelphia, PA	20	3	39 54 50/75 11 30
	Rotterdam Junction, NY	20	3	42 47 22/73 43 12
Schenectady	Oyster Creek, TX	50	8	29 58 21/95 20 38
	Total	300	48	

(continued)

TABLE E-79 (continued)

Company	Location	1978 capacity, 10^6 lb/yr	1978 production, 10^6 lb/yr	Geographical location, latitude/longitude
Salicylic acid producers				
Dow	Midland, MI	15	14	43 35 28/84 13 08
Monsanto	St. Louis, MO	20	18	38 34 37/90 11 42
Sterling Drug	Cincinnati, OH	8	7	39 05 15/84 33 09
Tenneco	Garfield, NJ	10	9	40 52 28/74 06 49
	Total	53	48	
Dodecylphenol producers				
Borg Warner	Morgantown, WV	60	4	39 40 39/80 58 34
GAF	Calvert City, KY	5	1	37 02 05/88 21 12
Monsanto	Kearney, NJ	40	9	40 46 12/74 09 08
	Total	105	14	
Adipic acid producer				
Allied	Hopewell, VA	30	24	37 22 13/77 18 08
	Total	30	24	

Source: Systems Applications, Inc. 1980.

TABLE E-80. PHENOL EMISSIONS FROM PHENOL PRODUCERS

Company	Location	Process emissions, lb/yr	Storage emissions, lb/yr	Fugitive emissions, lb/yr	Total emissions lb/yr	Total emissions g/s
Allied	Philadelphia, PA	23,000	172,000	12,740	207,740	2.99
Clark	Blue Island, IL	117,480	1,980	27,060	146,520	2.11
Dow	Freeport, TX	624,780	10,530	143,910	779,220	11.22
Georgia Pacific	Plaquemine, LA	356,000	6,000	82,000	444,000	6.39
Getty	El Dorado, KS	128,160	2,160	29,520	159,840	2.30
Kalama	Kalama, WA	101,460	1,710	23,370	126,540	1.82
Monsanto	Chocolate Bayou, TX	8,419	142	1,939	10,500	.15
Shell	Deer Park, TX	671,060	11,310	154,570	836,940	12.05
Standard Oil of California	Richmond, CA	74,760	1,260	17,220	93,240	1.34
Union Carbide	Bound Brook, NJ	240,300	4,050	55,350	299,700	4.31
U.S. Steel	Haverhill, OH	436,100	7,350	100,450	543,900	7.83
Ferro	Sante Fe Springs, CA	9,612	162	2,214	11,988	0.17
Koppers	Follansbee, WV	9,612	162	2,214	11,988	0.17
Merichem	Houston, TX	9,612	162	2,214	11,988	0.17
Stimson	Anacortes, WA	9,612	162	2,214	11,988	0.17
U.S. Steel	Clairton, PA	9,612	162	2,214	11,988	0.17
Total		2,829,579	219,302	659,199	3,708,080	

Source: Systems Applications, Inc. 1982.

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TABLE E-81.   PHENOL PRODUCTION AND END-USE EMISSION FACTORS

| Source | Emission factor, lb phenol lost per lb used (produced) | | | | |
	Process	Storage	Fugitive	Total	Derivation[a]
Phenol production	0.00178	0.00003	0.00041	0.00222	C
Caprolactam	0.00130	0.00001	0.00013	0.00144	A
Bisphenol-A	0.00035	0.00003	0.00012	0.00050	C
Nonylphenol	0.00080	0.00001	0.00019	0.00100	C
Salicylic acid	0.00035	0.00001	0.00014	0.00050	C
Dodecylphenol	0.00080	0.00001	0.00019	0.00100	D
Phenolic resins	0.00035	0.00002	0.00013	0.00050	D
Adipic acid	Phenol emissions are included with caprolactam production losses				
Miscellaneous				0.00068[b]	

[a] A - Site visit data, B - State files, C - Published data, D - Hydroscience estimate

[b] Based on a weighted average of all other phenol end-use emission factors.

Source: Systems Applications, Inc. 1980.

TABLE E-82. PHENOL EMISSIONS FROM END USERS

Company	Location	Process lb/yr	Storage lb/yr	Phenol emissions Fugitive lb/yr	Total lb/yr	Total g/s
Bisphenol-A producers						
Dow	Freeport, TX	33,250	2,850	11,400	47,500	0.68
General Electric	Mount Vernon, IN	49,000	4,200	16,800	70,000	1.01
Shell	Deer Park, TX	33,250	2,850	11,400	47,500	0.68
U.S. Steel	Haverhill, OH	26,250	2,250	9,000	37,500	0.54
Total		141,750	12,150	48,600	202,500	
Caprolactam producer						
Allied	Hopewell, VA	461,500	3,550	46,150	511,200	7.36
Nonylphenol producers						
Borg Warner	Morgantown, WV	8,000	100	1,900	10,000	0.144
Exxon	Bayway, NJ	450	28	522	1,000	0.014
GAF	Calvert City, KY	800	10	190	1,000	0.014
	Linden, NJ	2,400	30	570	3,000	0.043
Jefferson	Port Neches, TX	4,800	60	1,140	6,000	0.086
Kalama	Kalama, WA	2,400	30	570	3,000	0.043
	Kearny, NJ	1,360	17	323	1,700	0.024
Monsanto	Deer Park, TX	1,600	20	380	2,000	0.029
Rohm and Haas	Philadelphia, PA	2,400	30	570	3,000	0.043

(continued)

TABLE E-82 (continued)

Company	Location	Phenol emissions				
		Process lb/yr	Storage lb/yr	Fugitive lb/yr	Total lb/yr	Total g/s
Nonylphenol producers (continued)						
Schenectady	Rotterdam Junction, NY	2,400	30	570	3,000	0.043
	Oyster Creek, TX	6,400	80	1,520	8,000	0.115
	Total	33,010	435	8,255	41,700	
Salicylic acid producers						
Dow	Midland, MI	4,900	140	1,960	7,000	0.101
Monsanto	St. Louis, MO	6,300	180	2,520	9,000	0.130
Sterling Drug	Cincinnati, OH	2,450	70	980	3,500	0.050
Tenneco	Garfield, NJ	3,150	90	1,260	4,500	0.065
	Total	16,800	480	6,720	24,000	
Dodecylphenol producers						
Borg Warner	Morgantown, WV	11,200	140	2,660	14,000	0.202
GAF	Clavert City, KY	800	10	190	1,000	0.014
Monsanto	Kearny, NJ	7,200	90	1,710	9,000	0.130
	Total	19,200	240	4,560	24,000	
Adipic acid producer						
Allied	Hopewell, VA	Emissions are included in caprolactam production losses				

Source: Systems Applications, Inc. 1982.

TABLE E-83. EMISSIONS AND METEOROLOGICAL STATIONS OF SPECIFIC POINT SOURCES OF PHENOL

No.	Company	Site	Latitude	Longitude	Star station	Plant type[a]	Source type[b]	Emissions, g/s Process	Storage	Fugitive
1	Allied	Frankford, PA	40 18 15	079 52 43	14762	1	1	11.611296	0.195696	2.674512
2	Clark	Blue Island, IL	41 39 21	087 41 56	14855	1	1	1.691712	0.028512	0.389664
3	Georgia Pacific	Plaquemine, LA	30 15 00	091 11 00	13970	1	1	5.126400	0.086400	1.180800
4	Getty	El Dorado, KS	37 47 10	096 52 00	03920	1	1	1.845504	0.031104	0.425088
5	Monsanto	Chocolate Bayou, TX	29 14 55	095 12 45	12906	1	1	9.663264	0.162864	2.225808
6	Standard	Richmond, CA	37 56 12	122 20 48	12906	1	1	1.076544	0.018144	0.247968
7	Union Carbide	Bound Brook, NJ	40 33 32	074 31 18	94741	1	1	3.468320	0.058320	0.797040
8	Ferro	Sante Fe Springs, CA	33 56 30	118 04 18	93106	1	1	0.138413	0.002338	0.031882
9	Koppers	Follansbee, WV	40 23 10	080 35 07	14762	1	1	0.138413	0.002338	0.031882
10	Merichem	Houston, TX	29 45 36	095 10 48	12906	1	1	0.138413	0.002338	0.031882
11	Stimson	Anacortes, WA	48 28 31	122 32 48	24217	1	1	0.138413	0.002338	0.031882
12	U.S. Steel	Clairton, PA	40 18 15	079 52 43	14762	1	1	0.138413	0.002338	0.031882
13	Dow	Freeport, TX	28 59 30	095 23 35	12923	2	1 2	8.996832 0.478800	0.151632 0.041040	2.072304 0.164160
14	Shell	Deer Park, TX	29 43 30	095 06 15	12986	2	1 2	9.663264 0.478800	0.162864 0.041040	2.225888 0.164160
15	U.S. Steel	Haverhill, OH	38 34 53	083 49 36	13866	2	1	6.279840 0.378000	0.105840 0.032400	1.446480 0.129600

(continued)

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TABLE E-83 (continued)

No.	Company	Site	Latitude	Longitude	Star station	Plant type[a]	Source type[b]	Emissions, g/s Process	Storage	Fugitive
16	Kalama	Kalama, WA	46 00 54	122 51 05	24229	3	1 4	1.461024 0.034560	0.024624 0.000432	0.836528 0.008208
17	General Electric	Mount Vernon, IN	37 56 43	087 34 25	93817	4	3	0.705600	0.060480	0.241920
18	Allied	Hopewell, VA	37 23 13	077 18 08	13740	5	3	6.643600	0.051120	0.664560
19	Exxon	Bayway, NJ	40 38 46	074 11 48	94741	6	4	0.034560	0.000432	0.008208
20	GAF	Linden, NJ	40 38 19	074 15 26	94741	6	4	0.034560	0.000432	0.008208
21	Jefferson	Port Neches, TX	29 57 45	093 56 00	12917	6	4	0.069120	0.000864	0.016416
22	Rohm and Haas	Deer Park, TX	29 43 00	095 06 15	12906	6	4	0.028040	0.000288	0.005472
23	Rohm and Haas	Philadelphia, PA	39 54 50	075 11 30	13739	6	4	0.034560	0.000432	0.008208
24	Schenectady	R Junction, NY	42 47 22	073 43 12	14735	6	4	0.034560	0.000432	0.008208
25	Schenectady	Oyster Creek, TX	29 58 21	095 20 38	12960	6	4	0.092160	0.001152	0.021888
26	Borg Warner	Morgantown, PA	39 40 39	080 58 34	13736	7	4 6	0.115200 0.161288	0.001440 0.002016	0.027360 0.038304
27	GAF	Calvert City, KY	37 02 50	088 21 12	03816	7	4 6	0.011520 0.011520	0.000144 0.000144	0.002736 0.002736
28	Monsanto	Kearny, NJ	40 46 12	074 09 08	94741	7	4 6	0.069120 0.103680	0.000864 0.001296	0.016416 0.024624
29	Dow	Midland, MI	43 35 28	084 13 08	14845	8	5	0.070560	0.002016	0.028224
30	Monsanto	St. Louis, MO	33 34 37	097 11 42	13994	8	5	0.090720	0.002592	0.036288
31	Sterling	Cincinnati, OH	39 05 15	084 33 09	13840	8	5	0.035280	0.001008	0.014112
32	Tenneco	Garfield, NJ	40 52 28	074 06 47	94741	8	5	0.045360	0.001296	0.018144

(continued)

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TABLE E-83 (continued)

a Plant types: 1 – plant produces phenol; 2 – plant produces phenol and Bisphenol-A; 3 – plant produces phenol and nonylphenol; 4 – plant produces Bisphenol-A; 5 – plant produces caprolactam and adipic acid; 6 – plant produces nonylphenol; 7 – plant produces nonylphenol and dodecylphenol; 8 – plant produces salicylic acid.

b Source types: 1 – phenol production; 2 – Bisphenol-A production; 3 – caprolactam/adipic acid production; 4 – nonylphenol production; 5 – salicylic acid production; 6 – dodecylphenol production.

Source: Systems Applications, Inc. 1982.

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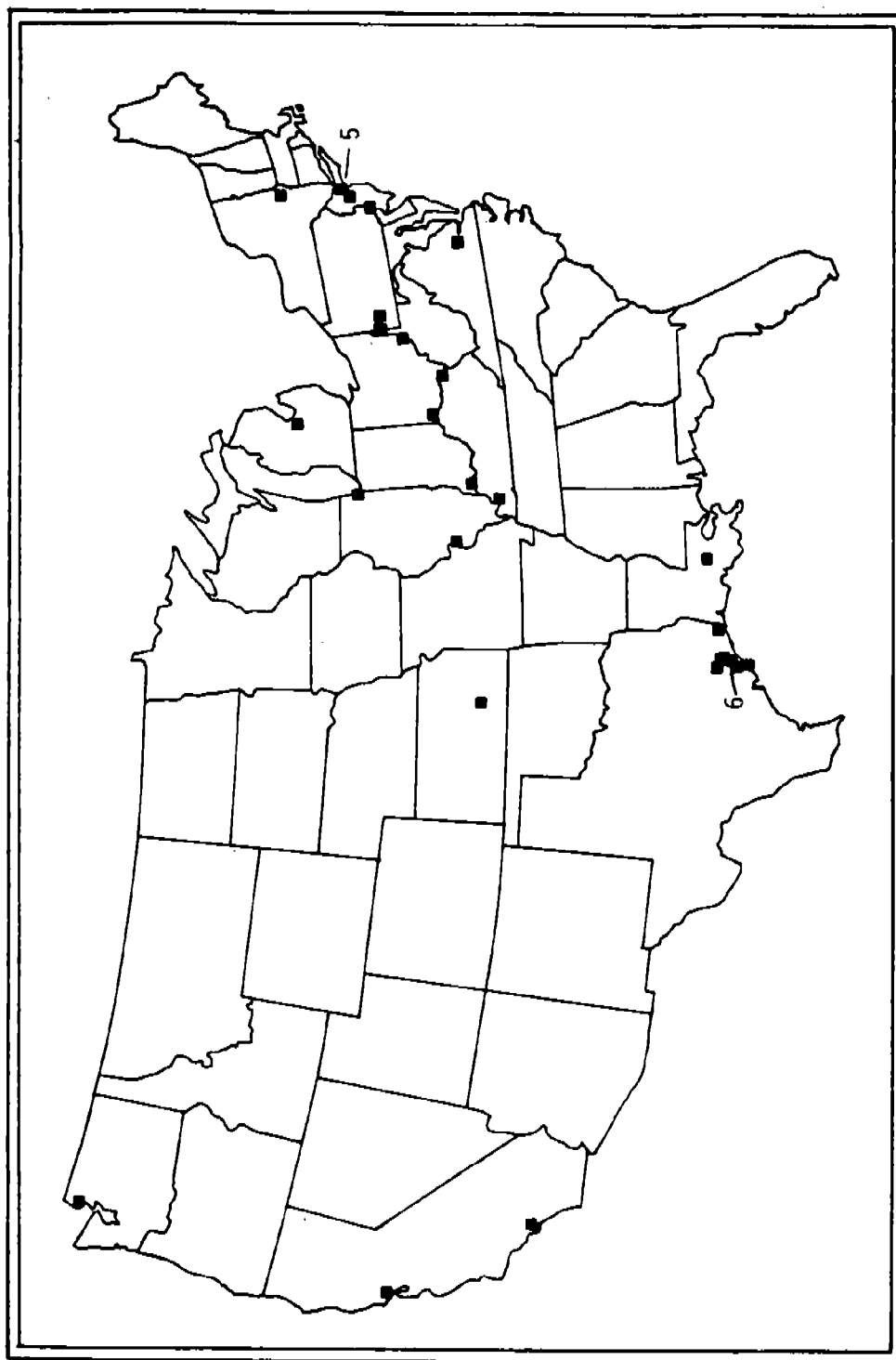
NOTE: NUMERALS DENOTE NUMBER OF PLANTS.

Figure E-5. Specific point sources of phenol emissions.

Source: Systems Applications, Inc. 1980.

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Storage:
    Should be protected from physical damage, and stored in a
    cool, dry, well-ventilated location, away from any areas where
    the fire hazard may be acute. Outside or detached storage is
    preferred, separate from other storage. Spills must be dis-
    posed of immediately by properly protected personnel.

Transportation:
    Should be shipped in bottles, cans, drums, tankcars, tank
    barges. Must be labled "Poison B."

Disposition:
    Phenol may be disposed of by incineration.

Sampling and Analytical Methods

1. NIOSH Method S330
    a. Bubbler (0.1 $\underline{N}$ sodium hydroxide).
    b. Gas chromatography.
    c. Flame ionization detector.

    Detection limit:
        0.25 ppm with 100-liter sample

    Possible interferences:
        None identified.

2. Method C (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar
    organics with boiling point between 60° and 200°C.
    a. Adsorption on Tenax.
    b. Thermal desorption.
    c. Gas chromatography/mass spectrometry analysis.

    Detection limit:
        1 to 200 ppt for a 20-liter sample

    Possible interferences:
        Blank levels usually limit sensitivity artifacts due to
        reactive components (O_3, NO_x). Sample can be analyzed
        only once.

3. Method S

Permissible Exposure Limits

	OSHA (skin)	ACGIH (skin)	NIOSH
TWA	5 ppm (19 mg/m³)	5 ppm (19 mg/m³)	20 mg/m³
STEL		10 ppm (38 mg/m³)	
Ceiling			60 mg/m³ (15 min)

Odor Perception: 0.022 mg/m³

Human Toxicity

Acute Toxicity:
Phenol vapor or liquid is readily absorbed through the skin or any mucous membrane, which may cause acute and chronic poisoning. A concentrated solution causes bad acid burns. Phenol is not sufficiently volatile to constitute a respiratory hazard under normal conditions. High toxicity for oral, intraperitoneal, subcutaneous, and parenteral methods. Moderate irritant to skin, subcutaneous, oral, and parenteral area. In acute poisoning, mainly effects central nervous system. Absorption from spilling phenolic solutions on skin may be very rapid, and death results from colapse within 30 minutes to several hours. Death has resulted from phenol absorption through 64 in.^{2} of skin area. Where death is delayed, damage to kidneys, liver, pancreas, and spleen; and edema of the lungs may result. Dermatitis resulting from contact with phenol or phenol-containing product is fairly common. As little as 1.5 g (oral) has killed.

Chronic Toxicity:
Phenol as a nonspecific irritant may promote development of tumors when applied repeatedly to the skin in large amounts. Results were negative in a carcinogenesis bioassay completed by the National Cancer Institute.

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Chemical Name

Phosgene

CAS Number

75-44-5

Chemical Classification

Chlorinated carbonyl

Synonyms

Carbone (oxychlorure de); carbon oxychloride; carbonylchlorid; carbonyl chloride; CG; chloroformyl chloride; carbino (ossichoruro di) diphosgene; fosgeen; fosgen; fosgene; koolstofoxychloride; NCI-60219; phosgen; phosgene (DOT)

Physical/Chemical Properties

Description:
Liquid or easily liquified gas; colorless to light yellow; odor varies from strong to stifling when concentrated to hay-like or diluted form.

Boiling Point:
8.2°C

Melting Point:
-128°C

Molecular weight:
98.9

Chemical Formula:
$COCl_2$

Vapor Pressure:
1180 mm at 20°C

Vapor Density:
3.4 (air = 1)

Refractive Index:
Not available

Solubility:
Slightly soluble in water and slowly hydrolized. Soluble in benzene and toluene.

Log Partition Coefficient (octanol/water):
Not available

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Photochemical Reactivity:
In the atmosphere, phosgene decomposes in water to form hydro-chloric acid.

Chemical Reactivity:
Decomposes in water to form hydrochloric acid. Because of its high degree of reactivity, phosgene interacts with many class-es of inorganic and organic reagents. Reacts violently with Al, tert-butyl azido formate, 2,4-hexadiyn-1,6-diol, isopropyl alcohol, K, Na, hexafluoro isopropylidene, amino lithium, lithium.

Environmental Fate
Rapid hydrolysis to CO_2 and HCl is the principal fate. Photolysis can occur, but cannot compete with hydrolysis.

Source of Emissions

Production:
Obtained by passing a mixture of carbon monoxide and chlorine over activated carbon.

Uses:
Organic synthesis, especially in isocyanates, polyurethane and polycarbonate resins, carbonates, organic carbonates, and chloroformates.
Pesticides
Herbicides
Dye manufacture

Tables E-84 through E-92 and Figure E-6 graphically present phosgene production, consumption, and emission data.

Storage:
Should be protected against physical damage and stored outdoors or in a well-ventilated area of noncombustible construction.

Transportation:
Should be shipped in steel cylinders and tank cars. All phosgene containers require "Poison A" labels.

Disposition:
Because of its low boiling point and high toxicity, phosgene should never be allowed to enter drains or sewers. If recycl-ing of phosgene is not feasible, phosgene waste can be handled by caustic scrubbing in packed columns.

Sampling and Analytical Methods

1. NIOSH Method 219
    a. Midget impinger.
    b. Nitrobenzylpyridine.
    c. Calorimetric analysis.

TABLE E-84. PHOSGENE PRODUCERS

Company	Location	1978 capacity, 10^6 lb/yr	1978 production, 10^6 lb/yr	Geographical location, latitude/longitude
Allied Chemical	Moundsville, WV	100	76	39 54 24/80 47 51
BASF Wyandotte	Geismar, LA	55	41.8	30 11 34/91 00 42
Chemtron	LaPorte, TX	80	60.8	29 39 20/95 02 18
Dow Chemical	Freeport, TX	130	98.8	28 59 12/95 24 05
DuPont	Deepwater, NJ	135	102.6	39 41 25/75 30 35
General Electric	Mt. Vernon, IN	60	45.6	37 56 42/87 54 25
Jefferson	Port Neches, TX	30	22.8	30 18 50/95 23 06
Minerec	Baltimore, MD	8	6.1	39 14 11/76 34 41
Mobay Chemical	Baytown, TX	250	190	29 45 30/94 54 25
	New Martinsville, WV	250	190	39 43 35/80 49 43
Olin	Ashtabula, OH	50	38	41 53 46/80 43 22
	Lake Charles, LA	120	91.2	30 13 55/93 15 57
PPG	Barberton, OH	5	3.8	41 00 37/81 36 29
Rubicon Chemicals	Geismar, LA	130	98.8	30 12 00/91 00 30
Stauffer Chemicals	Cold Creek, AL	25	19	30 58 30/88 01 16
Upjohn	LaPorte, TX	200	152	29 42 26/95 04 29
Van De Mark	Lockport, NY	8	6.1	43 11 08/78 42 40
Total		1,636	1,243.4	

Source: Systems Applications, Inc. 1982.

TABLE E-85. PHOSGENE END-USE DISTRIBUTION

Source	Usage, 10^6 lb/yr	Percent usage
Toluene diisocyanates (TDI)	814.5	60
Polymeric isocyanates (MDI)	339.5	25
Polycarbonates	67.8	5
Miscellaneous	135.6	10
Total	1357.4	100

Source: Systems Applications, Inc. 1980.

TABLE E-86. PHOSGENE USERS
(manufacturers of polymeric isocyanates)

Company	Location	1978 MDI capacity, 10^6 lb/yr	1978 phosgene use, 10^6 lb/yr	Geographical location, latitude/longitude
Mobay Chemical	Baytown, TX	110	81.25	29 45 30/94 54 25
	New Martinsville, WV	50	36.9	39 44 50/80 50 50
Rubicon Chemicals	Geismar, LA	50	36.9	30 12 00/91 00 30
Upjohn	LaPorte, TX	250	184.4	29 42 26/95 04 29
Total		460	339.5	

Source: Systems Applications, Inc. 1980.

TABLE E-87. PHOSGENE USERS
[manufacturers of toluene diisocyanate (TDI)]

Company	Location	1978 TDI capacity, 10^6 lb/yr	1978 phosgene use, 10^6 lb/yr	Geographical location, latitude/longitude
Allied Chemical	Moundsville, WV	80	80.9	39 54 39/80 44 49
BASF Wyandotte	Geismar, LA	100	101.2	30 11 34/91 00 42
Dow Chemical	Freeport, TX	100	101.2	28 59 12/95 24 05
DuPont	Deepwater, NJ	70	70.8	39 41 25/75 30 35
Mobay Chemical	Baytown, TX	130	131.5	29 45 30/94 54 25
	New Martinsville, WV	100	101.2	39 44 50/80 50 50
Olin	Ashtabula, OH	30	30.4	41 53 07/80 45 50
	Lake Charles, LA	100	101.2	30 13 55/93 15 57
Rubicon Chemicals	Geismar, LA	40	40.5	30 12 00/91 11 30
Total		750	758.9	

Source: Systems Applications, Inc. 1982.

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TABLE E-88. TOTAL PHOSGENE EMISSIONS FROM PRODUCERS AND USERS

Company	Location	Phosgene emissions	
		lb/yr	g/s
Allied Chemical	Moundsville, WV	14,214	0.204
BASF Wyandotte	Geismar, LA	8,190	0.118
Chemtron	LaPorte, TX	10,964	0.158
Dow Chemical	Freeport, TX	18,450	0.264
DuPont	Deepwater, NJ	18,934	0.273
General Electric	Mt. Vernon, IN	8,208	0.118
Jefferson	Port Neches, TX	4,104	0.059
Minerec	Baltimore, MD	1,098	0.016
Mobay Chemical	Baytown, TX	35,548	0.511
	New Martinsville, WV	35,086	0.505
Olin	Ashtabula, OH	7,020	0.101
	Lake Charles, LA	17,082	0.246
PPG	Barberton, OH	684	0.01
Rubicon Chemicals	Geismar, LA	18,270	0.263
Stauffer Chemicals	Cold Creek, AL	3,420	0.049
Union Carbide	S. Charleston, WV	20,086	0.30
Upjohn	LaPorte, TX	28,580	0.412
Van De Mark	Lockport, NY	1,098	0.016
Total		251,036	3,624

Source: Systems Applications, Inc. 1982.

TABLE E-89. SOURCES OF PHOSGENE EMISSIONS

Source	Production/usage, 10^6 lb/h	Percent usage	Total emissions lb/yr	Total emissions g/s
Producers	1357.4	-	190,960	2.749
Users:				
Toluene diisocyanate	746.0	60	4,998	0.078
Polymeric isocyanates	310.9	25	2,140	0.031
Polycarbonates	62.2	5	447[a]	0.006
Miscellaneous	124.3	10	893[a]	0.012
Total	2600.8	100	199,438	2.876

[a] Based on emission factor for toluene diisocyanate (TDI)

Source: Systems Applications, Inc. 1982.

TABLE E-90. PHOSGENE EMISSIONS FROM PHOSGENE USERS FOR MDI PRODUCTION

Company	Location	Process vent emissions lb/yr	Process vent emissions g/s	Fugitive emissions lb/yr	Fugitive emissions g/s	Total emissions lb/yr	Total emissions g/s
Mobay Chemical	Baytown, TX	480	0.007	Nil	Nil	480	0.007
	New Martinsville, WV	220	0.003	Nil	Nil	220	0.003
Rubicon Chemicals	Geismar, LA	220	0.003	Nil	Nil	220	0.003
Upjohn	LaPorte, TX	1220	0.018	Nil	Nil	1220	0.018
Total						2140	0.031

Source: Systems Applications, Inc. 1980.

TABLE E-91. PHOSGENE EMISSIONS FROM PHOSGENE USERS FOR TDI PRODUCTION

Company	Location	Process vent emissions		Fugitive emissions		Total emissions	
		lb/yr	g/s	lb/yr	g/s	lb/yr	g/s
Allied Chemical	Moundsville, WV	534	0.008	Nil	Nil	534	0.008
BASF Wyandotte	Geismar, LA	666	0.01	Nil	Nil	666	0.01
Dow Chemical	Freeport, TX	666	0.01	Nil	Nil	666	0.01
DuPont	Deepwater, NJ	466	0.007	Nil	Nil	466	0.007
Mobay Chemical	Baytown, TX	868	0.012	Nil	Nil	868	0.012
	New Martinsville, WV	666	0.01	Nil	Nil	666	0.01
Olin	Ashtabula, OH	200	0.003	Nil	Nil	200	0.003
	Lake Charles, LA	666	0.01	Nil	Nil	666	0.01
Rubicon Chemicals	Geismar, LA	266	0.004	Nil	Nil	266	0.004
Total						4,998	0.074

Source: Systems Applications, Inc. 1982.

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No.	Company	Site	Latitude	Longitude	Star station	Plant type[a]	Source type[b]	Emissions, g/s		
								Process	Storage	Fugitive
1	Allied Chemical	Moundsville, WV	39 54 39	080 44 49	13736	1	1	0.002442	0.	0.062437
2	BASF Wyandotte	Geismar, LA	30 11 34	091 00 42	13979	1	1	0.000349	0.	0.003964
3	Dow	Freeport, TX	28 59 30	095 23 35	12923	1	1	0.256089	0.	0.009576
4	DuPont	Deepwater, NJ	39 41 25	075 30 35	13739	1	1	0.006722	0.	0.265950
5	Mobay	Baytown, TX	29 45 30	094 54 25	12906	1	1	0.019502	0.	0.492485
6	Mobay	New Martinsville, WV	39 44 50	080 50 50	13736	1	1	0.492485	0.	0.012748
7	Olin	Astabula, OH	41 53 07	080 45 50	14843	1	1	0.002886	0.	0.098491
8	Olin	Lake Charles, LA	30 13 55	093 15 57	03937	1	1	0.000095	0.	0.002220
9	Rubicon	Geismar, LA	30 12 00	091 11 30	12958	1	1	0.007008	0.	0.256088
10	Upjohn	LaPorte, TX	29 42 36	095 04 29	12906	1	1	0.017567	0.	0.393994
11	Chemetron	LaPorte, TX	29 39 20	095 02 18	12906	2	1	0.	0.	0.151890
12	General Electric	Mt. Vernon, IN	37 56 42	087 34 25	93817	2	1	0.	0.	0.118182
13	Jefferson	Port Neches, TX	29 57 45	093 56 00	12917	2	1	0.	0.	0.059107
14	Minerec	Baltimore, MD	39 14 11	076 34 41	13701	2	1	0.	0.	0.015823
15	ITC	Barberton, OH	41 00 37	081 36 29	14095	2	1	0.	0.	0.009323
16	Stauffer	Cold Creek, AL	30 58 30	088 01 16	93841	2	1	0.	0.	0.049245
17	Vandermark	Lockport, NY	43 11 08	078 42 40	14747	2	1	0.	0.	0.015823

[a] Plant types: 1 - plant produces and consumes phosgene; 2 - plant produces phosgene.
[b] Source types: 1 - phosgene production/consumption processes.

Source: Systems Applications, Inc. 1980.

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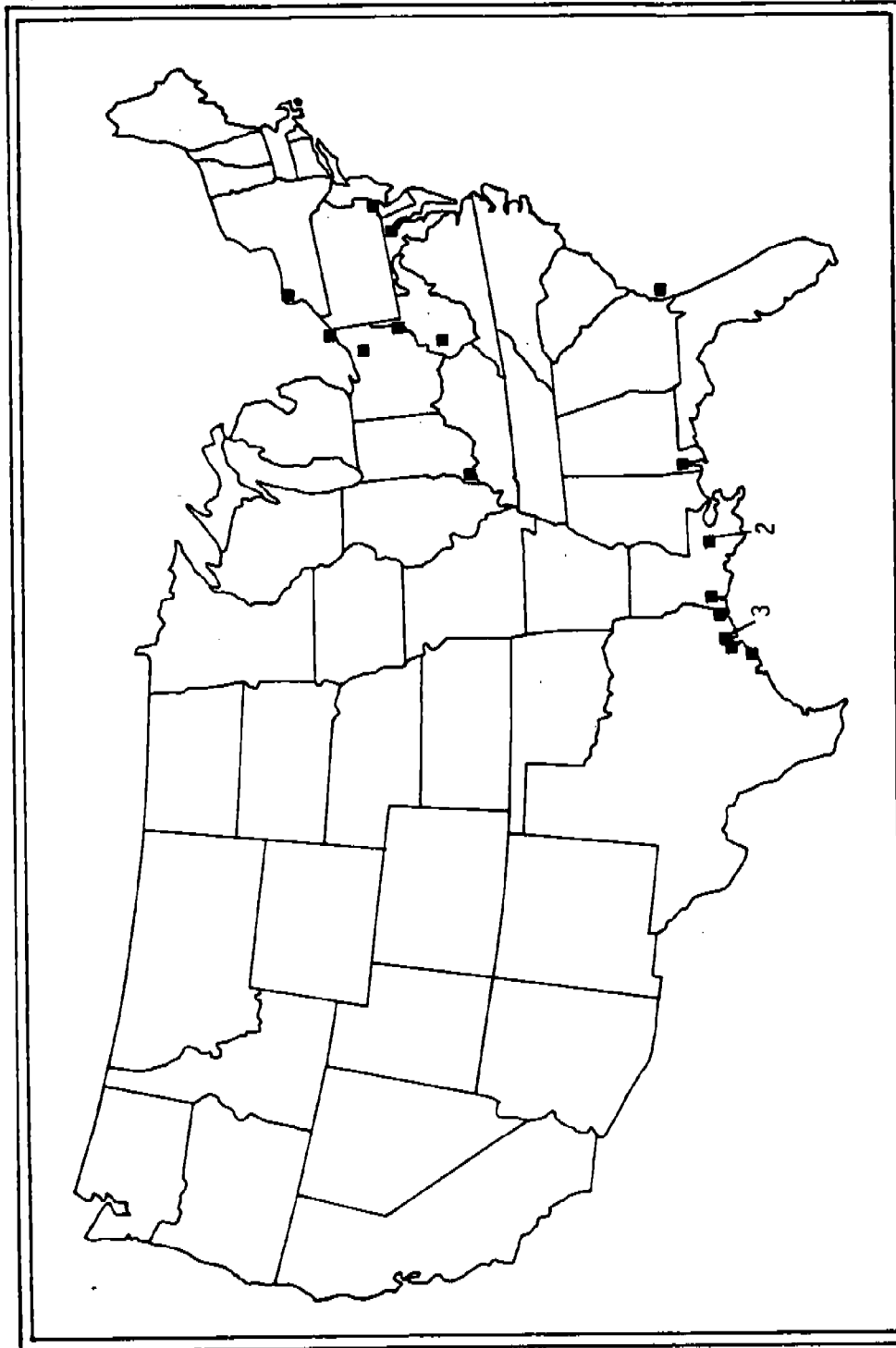
NOTE: NUMERALS DENOTE NUMBER OF PLANTS.

Figure E-6. Specific point sources of phosgene emissions.

Source: Systems Applications, Inc. 1980.

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Detection limit:
    0.005 ppm with a 250-liter sample

Possible interferences:
    Other acid chlorides, alkyl and aryl derivatives that are
    substituted by active halogen atoms, and sulfate esters
    are known to produce color with this reagent.

Because this compound is highly unstable, a field determination
should be made. A manual colorimetric test using 4-nitrobenzyl-
pyridine appears to be the best approach for routine analysis
(detection limit approximately 0.05 ppm for 25-liter sample).

Permissible Exposure Limits

	OSHA	ACGIH	NIOSH
TWA	0.1 ppm (0.4 mg/m³)	0.1 ppm (0.4 mg/m³)	0.1 ppm
Ceiling			0.2 ppm

Odor Perception 0.5 to 1 ppm.

Human Toxicity

Acute Toxicity:
    High toxicity via inhalation. High irritant to eyes and
    mucous membrane at 4 ppm. In presence of moisture, phosgene
    decomposes to form hydrochloric acid and carbon monoxide.
    This action takes place within the body when the gas reaches
    the bronchioles and the alevoli of the lungs. There is little
    irritation effect upon the respiratory tract; therefore, the
    warning properties of the gas are very slight. Concentrations
    of 3 to 5 ppm of phosgene in air cause irritation of the eyes
    and throat, with coughing; 25 ppm is dangerous for exposure
    lasting 30 to 60 minutes; and 50 ppm is rapidly fatal even
    after short exposure.

Chronic Toxicity:

    Epidemiologic studies have shown no ill effects definitely
    attributable to phosgene in 326 workers exposed to an average
    of 0.125 ppm or less for considerable periods.

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    Work Environment and Biological Exposure Indices With Intended Changes for
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Chemical Name

Propylene oxide

CAS Number

75-56-9

Chemical Classification

Epoxide

Synonyms

Epoxypropane; 1,2-epoxypropane; ethylene oxide, methyl; methyl ethylene oxide; methyl oxirane; NCI-50099; oxirane, methyl; oxyde de propylene; propane, epoxy-; propene oxide; propylene oxide; 1,2-propylene oxide; propylene oxide (DOT).

Physical/Chemical Properties

Description:
Colorless liquid; ethereal odor.

Boiling Point:
33.9°C

Melting Point:
-104.4°C

Molecular Weight:
58.8

Chemical Formula:
$CH_2-CH-CH_3$

Vapor Pressure:
445 mm (20°C)   400 mm at 17.8°C

Vapor Density:
2.0 (air = 1)

Refractive Index:
N_D^{20} = 1.3670

Solubility:
Partially soluble in water, soluble in alcohol and ether.

Log Partition Coefficient (octanol/water):
Not available

Photochemical Reactivity:
    Not available

Chemical Reactivity:
    Reacts with active hydrogen compounds (e.g., alcohols, amines)
    and with inorganic chloride in foods to form 1-chloro-2-
    propanol. Also reacts with 4-(4'-nitrobenzyl)pyridine.
    Violent reaction with NH_4OH, chlorosulfonic acid, HCl, HF,
    HNO_3, oleum, and H_2SO_4.

Environmental Fate
    Propylene oxide exhibits a high degree of reactivity with a large
    number of chemicals including water.

Source of Emissions

    Production:
        Chlorohydration of propylene, followed by saponification with
        lime.
        Peroxidation of propylene.
        Epoxidation of propylene by a hydroperoxide complex with
        molybdenum catalyst.

    Uses:
        Polyols for urethane foams
        Propylene glycols
        Surfactants and detergents
        Isopropanol amines
        Fumigant
        Synthetic lubricants
        Synthetic elastomer (homopolymer)
        Solvent

        Tables E-93 through E-105 and Figure E-7 present propylene
        oxide production, consumption, and emission data.

    Storage:
        Carbon steel or stainless steel should be used. Teflon-filled
        spiral-wound stainless steel or glass-filled Teflon can be
        used for gaskets or seals. Should be protected against physi-
        cal damage. Detached outside storage is preferred. Inside
        storage should be in a standard flammable liquids storage room
        or cabinet. Keep isolated from combustible materials and
        oxidizing agents. Propylene oxide tanks should be insulated,
        protected by sprinklers, diked, and electrically grounded. An
        inert gas such as nitrogen or methane should be kept over the
        oxide during storage and transfer.

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TABLE E-93. PROPYLENE OXIDE PRODUCERS

Company	Location	1978 capacity, 10^6 lb/yr	Process[a]	1978 production,[b] 10^6 lb/yr	Geographical coordinates, latitude/longitude
BASF Wyandotte	Wyandotte, MI	175	A	109	42 12 55/83 08 35
Dow Chemical	Freeport, TX	1100	A	684	28 59 35/95 23 36
	Plaquemine, LA	340	A	212	30 19 00/91 15 32
Jefferson	Port Neches, TX	150	A	93	29 57 50/93 56 00
Olin	Brandenburg, KY	130	A	81	38 00 27/86 06 50
Oxirane	Bayport, TX	920	B	572	29 37 26/95 03 07
	Channelview, TX	400	B	249	29 48 50/95 07 30
Total		3215		2000	

[a] A = chlorohydrin
   B = peroxidation

[b] Based on 62.2% production to capacity ratio.

Source: Systems Applications, Inc. 1980.

TABLE E-94. PROPYLENE OXIDE END-USES 1978

Source	Usage, 10^6 lb/yr	Percent usage
Urethane polyols	1120	56
Propylene glycol	480	24
Surfactant polyols	120	6
Dipropylene glycol	100	5
Glycol ethers	40	2
Miscellaneous	40	2
Exports	100	5
Total	2000	100

Source: Systems Applications, Inc. 1980.

TABLE E-95. PROPYLENE OXIDE USERS FOR GLYCOL ETHERS PRODUCTION

Company	Location	Propylene oxide used,[a] 10^6 lb/yr	Geographic location, latitude/longitude
Dow Chemical	Freeport, TX	19.5	28 59 35/95 23 36
	Plaquemine, LA	13.0	30 19 00/91 15 32
Olin	Brandenburg, KY	7.5	38 08 27/86 06 50
	Total	40.0	

[a] Propylene oxide use allocated over the three sites based on ethylene glycol ethers capacity in the absence of propylene glycol ether figures.

Source: Systems Applications, Inc. 1980.

TABLE E-96. PROPYLENE OXIDE USERS FOR URETHANE POLYOLS PRODUCTION

Company	Location	1978 urethane polyols capacity, 10⁶ lb/yr	1978 propylene oxide used, 10⁶ lb/yr	Geographical coordinates, latitude/longitude
BASF Wyandotte	Geismar, LA	100	45	30 11 34/91 00 42
	Washington, NJ	40	18	40 45 20/74 58 22
	Wyandotte, MI	225	101	42 12 55/83 08 35
E. R. Carpenter Co.	Bayport, TX	150	68	29 43 20/94 54 00
Dow Chemical	Freeport, TX	400	180	28 59 35/95 23 36
	Midland, MI	20	9	43 34 08/84 16 26
Emery Industries	Mauldin, SC	10	4.5	34 48 16/82 16 09
	Santa Fe Springs, CA	10	4.5	33 55 30/118 05 40
Hodag Chemical Co.	Skokie, IL	10	4.5	42 01 50/87 43 39
Magna Corporation	Houston, TX	12	5	29 40 10/95 23 30
Milliken	Inman, SC	3	1.5	34 56 10/82 06 29
3M	Decatur, AL	15	7	34 38 39/87 02 25
Mobay Chemical	Baytown, TX	100	45	29 45 30/94 54 25
	New Martinsville, WV	80	36	39 44 50/80 50 55
Malco Chemical Co.	Sugar Land, TX	40	18	29 37 10/95 38 32
Olin Corporation	Brandenburg, KY	220	100	38 08 27/86 06 50
	Lake Charles, LA	30	14	30 13 85/93 15 57
Owens-Corning	Newark, OH	10	4.5	40 05 30/82 26 00
Pelron Corporation	Lyons, IL	22	10	41 44 56/87 49 04
Petrolite Corp.	Brea, CA	15	7	33 53 30/117 58 45
	St. Louis, MO	15	7	38 41 50/90 12 08
PPG Industries, Inc.	Circleview, OH	30	14	39 36 05/82 57 34
The Quaker Oats Co.	Memphis, TN	10	4.5	35 10 30/90 56 56
Reichold	Carteret, NJ	20	9	40 35 56/74 13 13
Jefferson Chemical Co.	Austin, TX	33	15	30 20 00/97 14 15
	Conroe, TX	33	15	30 18 50/95 23 06
	Port Neches, TX	34	15	29 57 50/93 56 00

(continued)

TABLE E-96 (continued)

Company	Location	1978 urethane polyols capacity, 10^6 lb/yr	1978 propylene oxide used, 10^6 lb/yr	Geographical coordinates, latitude/longitude
Union Carbide	Institute, WV	245	110	38 23 02/81 47 24
	Seadrift, TX	245	110	28 30 31/96 46 18
	S. Charleston, WV	250	113	38 22 13/81 40 44
	LaPorte, TX	14	6	29 42 44/95 04 45
Upjohn	Clearing, IL	25	11	41 48 02/87 46 39
Witco	Houston, TX	18	8	29 34 45/95 26 00
Total		2484	1120	

TABLE E-97. PROPYLENE OXIDE USERS FOR DIPROPYLENE AND TRIPROPYLENE GLYCOL PRODUCTION

Company	Location	Dipropylene glycol/tripropylene glycol production capacity, 10^6 lb/yr	Propylene oxide used, 10^6 lb/yr [a]	Geographical coordinates, latitude/longitude
Dow Chemical	Freeport, TX Plaquemine, LA	27.5 17.6	32.3 20.7	28 59 35/95 23 36 30 19 00/91 15 32
Olin	Brandenburg, KY	5	5.9	38 08 27/86 06 50
Oxirane	Bayport, TX	18	21.1	29 37 26/95 03 07
Jefferson	Port Neches, TX	7	8.2	29 57 50/93 56 00
Union Carbide	Institute, WV S. Charleston, WV	5[b] 5[b]	5.9 5.9	38 23 02/81 47 24 38 22 13/81 40 44
Total		85.1	100.0	

[a] Total propylene oxide used allocated per site based on the rate of dipropylene/tripropylene glycol individual site production capacity to total industry production capacity.

[b] Capacity of 10 million lb/yr equally distributed between the two sites.

Source: Systems Applications, Inc. 1980.

TABLE E-98. PROPYLENE OXIDE USERS FOR SURFACTANT POLYOLS PRODUCTION

Company	Location	Polyether polyols capacity, 10^6 lb/yr	Propylene oxide used,[a] 10^6 lb/yr	Geographical coordinates, latitude/longitude
Emery Industries	Sante Fe Springs, CA	10	2	33 55 30/118 05 40
Olin	Brandenburg, KY	270	51	38 08 26/86 06 50
Petrolite	Brea, CA	15[b]	3	33 53 30/117 58 45
	St. Louis, MO	15[b]	3	38 41 50/90 12 08
Sherex	Janesville, WI	5	1	42 40 47/89 00 30
Union Carbide	Institute, WV	100[c]	19	38 23 02/81 47 24
	Seadrift, TX	100[c]	19	28 30 31/96 46 18
	S. Charleston, WV	100[c]	19	38 22 13/81 40 44
Witco	Houston, TX	18	3	29 34 45/95 26 00
	Total	633	120	

[a] Total propylene oxide used distributed over each site based on polyether polyols capacity.

[b] Total capacity of 30 million lb equally distributed between both sites.

[c] Total capacity of 300 million lb equally distributed between all three sites.

Source: Systems Applications, Inc. 1980.

TABLE E-99. PROPYLENE OXIDE USERS FOR PROPYLENE GLYCOL PRODUCTION

Company	Location	1978 propylene glycol capacity, 10^6 lb/yr	1978 propylene oxide used,[a] 10^6 lb/yr	Geographical coordinates, latitude/longitude
Dow Chemical	Freeport, TX	250	140	28 59 35/95 23 36
	Plaquemine, LA	160	91	30 19 00/91 15 32
Jefferson	Port Neches, TX	50	28	29 57 50/93 56 00
Olin	Brandenburg, KY	45	25	38 08 27/86 06 50
Oxirane	Bayport, TX	250	140	29 37 26/95 03 07
Union Carbide	Institute, WV	50	28	38 23 02/81 47 24
	S. Charleston, WV	50	28	38 22 13/81 40 44
Total		855	480	

Source: Systems Applications, Inc. 1980.

TABLE E-100. 1978 PROPYLENE OXIDE NATIONWIDE EMISSIONS

Source	Estimated 1978 emissions, lb/yr
Production	1,160,660
Urethane polyols	147,840
Propylene glycol	13,920
Surfactant polyols	15,840
Dipropylene/tripropylene glycols	2,900
Glycol ethers	1,160
Miscellaneous	3,840[a]
Exports	0
Total	1,346,160

[a] Derived based on weighted average of other users except exports.

Source: Systems Applications, Inc. 1980.

TABLE E-101. EMISSIONS FROM DIPROPYLENE GLYCOL, TRIPROPYLENE GLYCOL, AND GLYCOL ETHER PRODUCERS

Company	Location	Process vent emissions, lb/yr	Fugitive emissions, lb/yr	Total emissions	
				lb/yr	g/s
Dow Chemical	Freeport, TX	1450	50	1500	0.022
	Plaquemine, LA	945	35	980	0.014
Jefferson	Port Neches, TX	230	10	240	0.003
Olin	Brandenburg, KY	375	15	390	0.006
Oxirane	Bayport, TX	590	20	610	0.009
Union Carbide	Institute, WV	165	5	170	0.002
	S. Charleston, WV	165	5	170	0.002
	Total	3920	140	4060	

Source: Systems Applications, Inc. 1980.

TABLE E-102. EMISSIONS FROM SURFACTANT POLYOL PRODUCERS

Company	Location	Process emissions, lb/yr	Storage emissions, lb/yr	Fugitive emissions, lb/yr	Total emissions	
					lb/yr	g/s
Emery	Santa Fe Springs, CA	260	Nil	Nil	265	0.004
Olin	Brandenburg, KY	6,630	50	50	6,730	0.097
Petrolite	Brea, CA St. Louis, MO	390 390	Nil Nil	Nil Nil	395 395	0.006 0.006
Sherex	Janesville, WI	130	Nil	Nil	130	0.002
Union Carbide	Institute, WV Seadrift, TX S. Charleston, WV	2,470 2,470 2,470	20 20 20	20 20 20	2,510 2,510 2,510	0.036 0.036 0.036
Witco	Houston TX	390	Nil	Nil	395	0.006
Total		15,600	110	110	15,840	

Source: Systems Applications, Inc. 1982.

TABLE E-103. EMISSIONS FROM PROPYLENE OXIDE USERS FOR PROPYLENE GLYCOL PRODUCTION

Company	Location	Process vent emissions, lb/yr	Fugitive emissions, lb/yr	Total emissions	
				lb/yr	g/s
Dow Chemical	Freeport, TX	3,920	140	4,060	0.058
	Plaquemine, LA	2,550	90	2,640	0.038
Jefferson	Port Neches, TX	785	30	815	0.012
Olin	Brandenburg, KY	700	25	725	0.010
Union Carbide	Institute, WV	785	30	815	0.012
	S. Charleston, WV	785	30	815	0.012
	Total	9,525	345	9,870	

Source: Systems Applications, Inc. 1982.

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TABLE E-104. EMISSIONS FROM PROPYLENE OXIDE USERS FOR URETHANE POLYOLS PRODUCTION[a]

Company	Location	Process vent emissions		Storage vent emissions		Fugitive emissions	Total emissions	
		lb/yr	g/s	lb/yr	g/s	lb/yr	lb/yr	g/s
BASF Wyandotte	Geismar, LA	103,703	1.49	708	0.10	40		
	Washington, NJ	2,400	0.03	20		20		
	Wyandotte, MI	13,200	0.19	100	0.002	80		
E. R. Carpenter Co.	Bayport, TX	8,800	0.13	80	0.001	60		
Dow Chemical	Freeport, TX	23,400	0.34	100	0.002	140		
	Midland, MI	1,200	0.02					
Emery Industries	Mauldin, SC	600	0.01					
	Santa Fe Springs, CA	600	0.01					
Hodag Chemical Co.	Skokie, IL	600	0.01					
Magna Corporation	Houston, TX	600	0.01					
Milliken	Inman, SC	200						
Minnesota Mining & Manufacturing	Decatur, AL	1,000	0.01					
Mobay Chemical	Baytown, TX	5,800	0.08	40	0.001	40		
	New Martinsville, WV	4,600	0.07	40	0.001	20		
Nalco Chemical Co.	Sugar Land, TX	2,400	0.03	20		20		
Olin	Brandenburg, KY	12,800	0.19	100	0.002	80		
Owens-Corning	Newark, OH	600	0.01					
Pelron Corporation	Lyons, IL	1,400	0.02	20				
Petrolite Corp.	Brea, CA	1,000	0.01					
PPG Industries, Inc.	St. Louis, MO	1,000	0.01					
The Quaker Oats Co.	Circleview, OH	1,800	0.03	20		20		
Reichold	Memphis, TN	600	0.01					
Jefferson Chemical Co.	Carteret, NJ	1,200	0.02					
	Austin, TX	2,000	0.03	20		20		
	Conroe, TX	2,000	0.03	20		20		
Union Carbide	Port Neches, TX	2,000	0.03	20		20		
	Institute, WV	14,300	0.21	120	0.002	80		
	Seadrift, TX	14,300	0.21	120	0.002	80		
	S. Charleston, WV	14,600	0.21	120	0.002	80		
Upjohn	LaPorte, TX	800	0.01	20		80	800	0.01
Witco	Clearing, IL	1,400	0.02				1,420	0.02
	Houston, TX	1,000	0.01				1,000	0.01
Total		241,903		1,688		820	244,411	

TABLE E-105. EMISSIONS FROM PROPYLENE OXIDE PRODUCERS

| Company | Location | Process vents[a] | | | | Storage vent emissions, lb/yr | Fugitive emissions, lb/yr | Total emissions | |
		Emissions, lb/yr	Stack height, m	Stack diameter, m	Stack temperature, °C			lb/yr	g/s
BASF Wyandotte	Wyandotte, MI	81,750	10.4	0.26	25	3,380	2,290	87,420	1.25
Dow Chemical	Freeport, TX	513,000	10.4	0.26	25	21,200	14,360	548,560	7.89
	Plaquemine, LA	159,000	10.4	0.26	25	6,570	4,450	170,020	2.45
Jefferson	Port Neches, TX	69,750	7.25	0.19	46	2,860	1,950	74,560	1.07
Olin	Brandenburg, KY	60,750	10.4	0.26	25	2,510	1,700	64,960	0.94
Oxirane	Bayport, TX	120,120	9.1	0.05	21	17,730	12,010	149,860	2.16
	Channelview, TX	52,290	14.6	0.76	26	7,720	5,230	65,240	0.94
Total		1,056,660				61,970	41,990	1,160,620	

[a] Stack velocity for all plants 2 m/s.

Source: Systems Applications, Inc. 1980.

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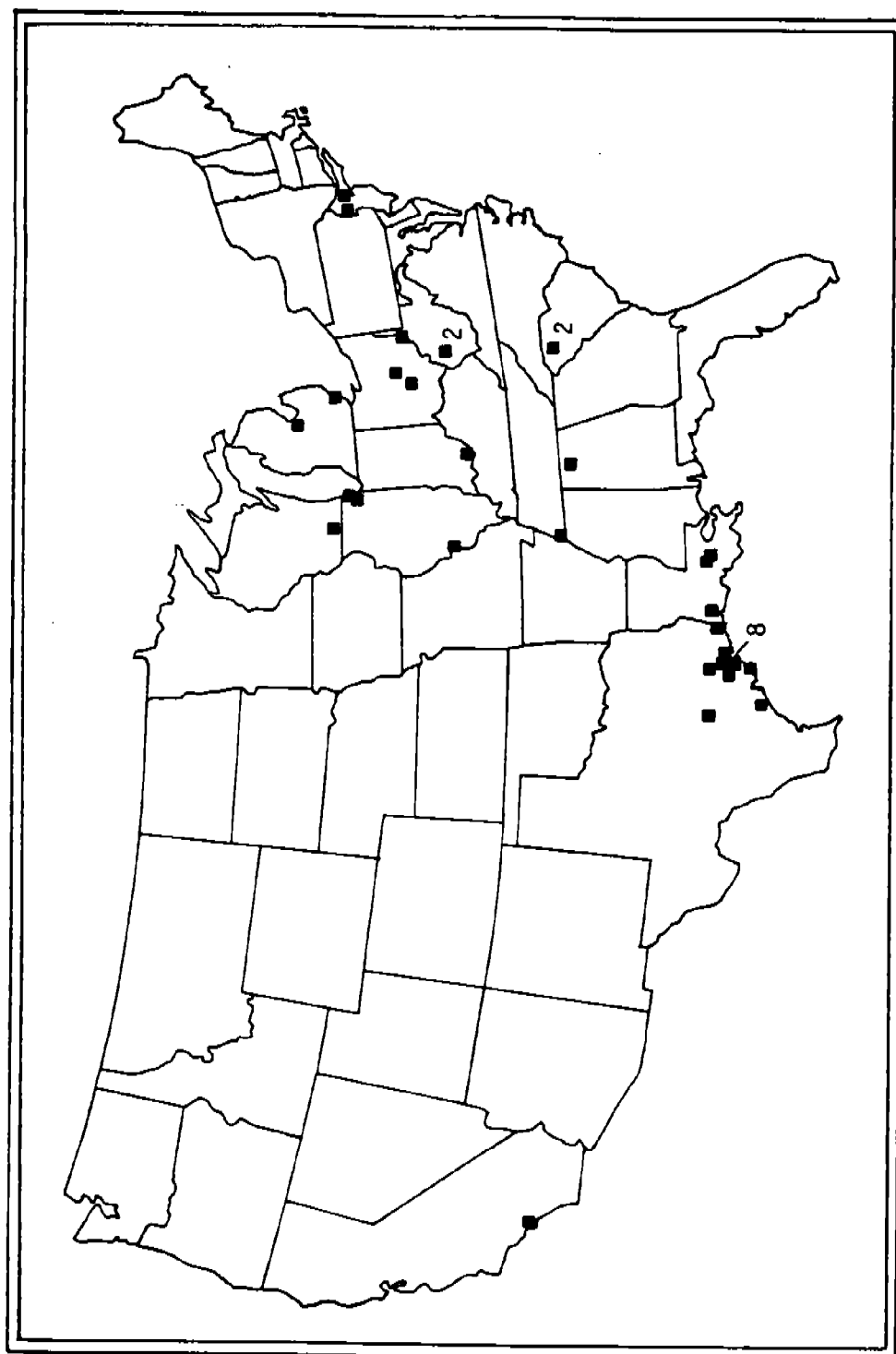
NOTE: NUMERALS DENOTE NUMBER OF PLANTS.

Figure E-7. Specific point sources of propylene oxide emissions.

Source: Systems Applications, Inc., 1980.

Transportation:
      Shipped in glass bottles, cans, metal drums, tank trucks, tank
      cars, tank barges, and cargo ships, usually with nitrogen over
      the propylene oxide. Must be labeled "Flammable Liquid."
      Shipment by ship must be kept under an inert gas pad and
      maintained at or below 40°C.

Disposition:
      Propylene oxide may be disposed of as a concentrated waste
      containing no peroxides by discharge of the liquid at a con-
      trolled rate near a pilot flame or as a concentrated waste
      containing peroxides by perforation of a container of the
      waste from a safe distance followed by open burning.

Sampling and Analytical Methods

Sampling and Analytical Methods

1. NIOSH Method S75
    a. Adsorption with charcoal.
    b. Desorption with carbon disulfide.
    c. Gas chromatography.

    Detection limit:
          25 to 720 mg/m³ (10 to 288 ppm) for a 5-liter sample

    Possible interferences:
          High humidity may hamper vapor trapping efficiency. Any
          compound with the same retention time as propylene oxide
          will cause interference.

2. Method B (Appendix A): C_2-C_{18} hydrocarbons and other nonpolar
    organics with a boiling point of 100° to 175°C.
    a. Whole air collection in canister.
    b. Cryogenic concentration.
    c. Gas chromatography/flame ionization detection.

    Detection limit:
          0.1 ppb per 100-ml sample

    Possible interferences:
          Water-soluble compounds are not readily analyzed. Stor-
          age times greater than a week are not recommended.

3. Method C (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with a boiling point between 60° and 200°C.
   a. Adsorption on Tenax.
   b. Thermal desorption.
   c. Gas chromatography/mass spectrometry analysis.

   Detection limit:
       1 to 200 ppt for a 20-liter sample

   Possible interferences:
       Blank levels usually limit sensitivity artifacts due to reactive components (O_3, NO_x). Sample can be analyzed only once. Low breakthrough volume on Tenex adsorption.

4. Method D (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with a boiling point of 60° to 200°C.
   a. Adsorption on Tenax.
   b. Thermal desorption into canisters.
   c. Gas chromatography/flame ionization detection, or gas chromatography/mass spectrometry analysis.

   Detection limit:
       0.01 to 1 ppb for a 20-liter sample

   Possible interferences:
       Blanks and artifact problems in Method C, above low breakthrough volume on Tenex adsorption.

Permissible Exposure Limits

	OSHA	ACGIH
TWA	100 ppm (240 mg/m³)	20 ppm (50 mg/m³)

Human Toxicity

Acute Toxicity:
    Skin and eye irritant. A food additive permitted in food for human consumption.

Chronic Toxicity:
    Propylene oxide was found to be carcinogenic in rats in a limited study in which subcutaneous injection produced sarcomas. No epidemiological studies were found.

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Chemical Name

o-, m-, p-xylene (where properties differ, they are presented in
o-, m-, p- order)

CAS Number

95-47-6; 108-38-3; 106-42-3; mixed isomers 1330-20-7

Chemical Classification

Aromatic hydrocarbon, alkyl benzene

Synonyms

(o-,m-,p-) dimethylbenzene; 1, (2-,3-,4-,) dimethylbenzene;
(o-,m-,p-,) methyltoluene; 1 (2-,3-,4-) xylene; (o-,m-,p-) xylol

Physical/Chemical Properties

Description:
Clear colorless liquid; p-xylene exists as crystals at low
temperature.

Boiling Point:
144°C; 138.8°C; 138.5°C

Melting Point:
-25°C; -47.4°C; 13.2°C

Molecular Weight:
106.2

Chemical Formula:
1, (2-,3-,4-) $C_6H_4(CH_3)_2$

Vapor Pressure:
10 mm Hg at 32.1°C; 10 mm Hg at 28.3°C; 10 mm Hg at 27.3°C

Vapor Density:
3.66 (air = 1.0)

Refractive Index:
$N_D^{20} = 1.505$; $N_D^{20} = 1.497$; $N_D^{20} = 1.500$

Solubility:
Soluble in alcohol and ether, insoluble in water.

Log Partition Coefficient (octanol/water):
2.77; 3.20; 3.15

Photochemical Reactivity:
    Transformation products are formaldehyde, acetaldehyde, PAN, and benzaldehyde. Xylene can be easily chlorinated, sulfonated, and nitrated. Reactivity toward OH· has a half-life of 3 days (8 times butane) for m and p; o has a half-life of 6 days. Reactivity toward O_3 has no reaction for o and m; half-life 100 years for p.

Chemical Reactivity:
    Contact with strong oxidizers may cause fires and explosions. Toxic gases and vapors (such as carbon monoxide) may be released in a fire involving xylene. Elevated temperatures may cause containers to burst. p-xylene incompatible with acetic acid + air; HNO_3; and 1,3-dichloro-3,5-dimethyl-2,4-imidazolidindione. Xylene will attack some forms of plastics, rubber, and coatings.

Environmental Fate

Calculated half-life in water at a depth of 1 meter at 25°C is 5.6 hours based on evaporative loss from the water. Some half-lives for photochemical reactions in air are presented in the photochemical reactivity section. Estimated overall lifetime under photochemical smog conditions in southeastern England is 2 to 6 hours.

Source of Emissions

Production:
    Selective crystallization or solvent extraction from meta-para mixtures.

Uses:
    Solvent
    Intermediate for dyes and organic synthesis especially for isophthalic acid
    Insecticides
    Aviation fuel

    Tables E-106 through E-119 and Figure E-8 present data on xylene production, consumption, and emissions.

Storage:
    Should be protected against physical damage. Outside or detached storage is preferable. Inside storage should be in a standard flammable liquids storage room or cabinet, separate from oxidizing materials.

Transportation:
    Shipped in glass containers in 55- and 110-gallon metal drums; in tank cars and tank trucks; and on tank barges.

Disposition:
    Xylenes may be disposed of by incineration

TABLE E-106. XYLENE ISOMER PRODUCERS

Company	Location	Isomer capacity, 10^6 lb/yr	Isomer production, 10^6 lb/yr	Geographic coordinates, Latitude/longitude
o-xylene Producers				
ARCO	Houston, TX	210	183	29 42 17/95 16 01
Corco	Ponce, PR	175	153	Not in project scope
Exxon	Baytown, TX	200	174	29 44 50/95 01 00
Monsanto	Chocolate Bayou, TX	30	26	29 14 55/95 12 45
Phillips	Guayama, PR	130	113	Not in project scope
Shell	Deer Park, TX	165	144	29 42 55/95 07 34
Sun	Corpus Christi, TX	160	140	27 49 53/97 31 30
Tenneco	Chalmette, LA	130	113	30 03 30/89 58 30
Total		1200	1046	
m-xylene Producer				
Amoco	Texas City, TX	175	88	29 21 40/94 55 50
p-xylene Producers				
Amoco	Decatur, AL	1300	952	34 36 12/86 58 42
	Texas City, TX	900	659	29 21 40/94 55 50
Arco	Houston, TX	360	264	29 42 17/95 16 01
Chevron	Pascagoula, MS	330	242	30 19 04/88 28 37
St. Croix	St. Croix, VI	600	440	Not in project scope

(continued)

TABLE E-106 (continued)

Company	Location	Isomer capacity, 10^6 lb/yr	Isomer production, 10^6 lb/yr	Geographic coordinates, latitude/longitude
p-xylene Producers (cont.)				
Exxon	Baytown, TX	420	308	29 44 50/95 01 00
Hercor	Penuelas, PR	600	440	Not in project scope
Phillips	Guayama, PR	470	344	Not in project scope
Shell	Deer Park, TX	110	80	29 42 55/95 07 34
Sun	Corpus Christi, TX	390	286	27 49 53/97 31 30
Tenneco	Chalmette, LA	125	92	30 03 30/89 58 30
Total		5605	4107	
Ethylbenzene Producers[a]				
ARCO	Houston, TX	136	99	29 42 17/95 16 01
Charter	Houston, TX	35	25	29 42 50/95 15 12
Monsanto	Chocolate Bayou, TX	59	43	29 14 55/95 12 45
Sun	Corpus Christi, TX	73	53	27 49 53/97 31 30
Total		303	220	

[a]Ethylbenzene is considered to be a mixed xylene isomer.

Source: Systems Applications, Inc., 1980.

TABLE E-107. MIXED XYLENE PRODUCTION SOURCE SUMMARY

Source	Isolated mixed xylene product, 10^6 lb/yr	Nonisolated mixed xylene production, 10^6 lb/yr	Total mixed xylene production, 10^6 lb/yr
Catalytic reformate	7,991	68,925	76,916
Pyrolysis gasoline	429	397	826
Toluene disproportionation	106	92	198
Coal-derived	29	4	33
Total	8,555	69,418	77,973

Source: Systems Applications, Inc., 1980.

TABLE E-108. ISOLATED MIXED XYLENE PRODUCTION FROM CATALYTIC REFORMATE

Company	Location	Mixed xylene capacity, metric tons/yr	Isolated mixed xylene produced, 10^6 lb/yr[b]	Geographic coordinates, Latitude/longitude
Amerada Hess	St. Croix, VI	457	699	Not in project scope
American Petrofina	Big Spring, TX	209	306	32 17 10/101 25 17
	Beaumont, TX	49	72	29 57 30/93 53 20
Ashland Oil	Catlettsburg, KY	98	143	38 22 39/82 35 58
	N. Tonawanda, NY	46	67	42 59 45/78 55 27
ARCO	Houston, TX	258	378	29 42 17/95 16 01
Charter Oil	Houston, TX	36	53	29 42 50/95 15 12
Cities Service	Lake Charles, LA	163	239	30 10 58/93 19 01
Coastal States	Corpus Christi, TX	55	80	27 48 43/97 26 28
Commonwealth	Penuelas, PR	343	502	Not in project scope
Crown	Pasadena, TX	46	67	29 44 40/95 10 30
Exxon	Baytown, TX	408	597	29 44 50/95 01 04
Gulf	Alliance, LA	196	287	29 50 00/90 00 10
Kerr McGee	Corpus Christi, TX	140	205	27 48 15/97 25 24
Marathon	Texas City, TX	36	53	29 22 22/94 54 58

(continued)

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TABLE E-108 (continued)

Company	Location	Mixed xylene capacity, metric tons/yr	Isolated mixed xylene produced, 10^6 lb/yr[b]	Geographic coordinates, Latitude/longitude
Monsanto	Texas City, TX	32	47	29 22 45/94 33 30
Phillips	Guayama, PR	326	477	Not in project scope
Quitana-Howell	Corpus Christi, TX	42	61	27 48 35/97 27 30
Shell	Deer Park, TX	245	359	29 42 55/95 07 33
Chevron	Pascagoula, MS	212	310	30 19 04/80 28 37
	Richmond, CA	196	287	37 56 12/122 20 48
Amoco	Texas City, TX	800	1,171	29 21 40/94 55 50
	Whiting, IN	588	860	41 41 07/87 29 02
Sun	Corpus Christi, TX	78	114	27 49 53/97 31 30
	Marcus Hook, PA	65	95	39 48 45/75 24 51
	Toledo, OH	163	239	41 36 52/83 31 40
Tenneco	Chalmette, LA	130	190	30 03 30/89 58 30
Union Oil	Chicago, IL	33	48	41 38 33/88 03 02
Union Pacific	Corpus Christi, TX	10	15	27 48 10/97 35 29
Total		5,460	8,021	

Source: Systems Applications, Inc., 1982.

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TABLE E-109. NONISOLATED MIXED XYLENE (AS BTX) PRODUCTION FROM
CATALYTIC REFORMATE

Region	Number of sites	Reformate capacity, 10^6 bbl/day	Non-isolated mixed xylene produced, 10^6 lb/yr	Average nonisolated mixed xylene produced per site, 10^6 lb/yr
New England	0	0	0	0
Middle Atlantic	17	369,952	6,743	397
East North Central	28	624,178	11,377	406
West North Central	16	165,250	3,012	188
South Atlantic	5	57,660	1,051	210
East South Central	8	144,700	2,637	330
West South Central	71	1,649,303	30,061	423
Mountain	23	123,094	2,243	98
Pacific	33	647,461	11,801	358
Total	201	3,781,598	68,925	343

Source: Systems Applications, Inc., 1980.

Company	Location	Production capacity, 10^6 lb/yr	Non-isolated mixed xylene produced, 10^6 lb/yr	Isolated mixed xylene produced, 10^6 lb/yr	Total mixed xylene produced, 10^6 lb/yr	Geographic coordinates, Latitude/longitude
Pyrolysis gasoline						
ARCO	Channelview, TX	1179	79	168	247	29 50 04/95 06 43
Commonwealth	Penuelas, PR	454	30	91	121	NA
Dow	Freeport, TX	1134	76		76	28 59 12/95 01 00
Exxon	Baton Rouge, LA	816	55		55	30 09 10/90 54 20
Gulf	Cedar Bayou, TX	544	37		37	29 49 29/94 55 10
Mobile	Beaumont, TX	408	27		27	30 04 00/94 03 30
Monsanto	Texas City, TX	340	23	61	84	29 15 00/95 12 40
Shell	Deer Park, TX	624	42		42	29 42 55/95 07 33
Union Carbide	Taft, LA	417	28	109	137	29 58 00/90 27 00
Total		5916	397	429	826	
Coal-derived						
Ashland	Catlettsburg, KY	13	1.6	11.4	13	38 22 39/82 35 58
	N. Tonawanda, NY	7	0.8	6.2	7	42 59 45/78 55 27
U.S. Steel	Clairton, PA	13	1.6	11.4	13	40 18 15/79 52 43
Total		33	4.0	29.0	33	
Toluene disproportionation						
ARCO	Houston, TX	196	45	52	97	29 42 17/95 16 01
Sun	Marcus Hook, PA	202	47	54	101	39 48 45/75 24 51
Total		398	92	106	198	

NA = Not applicable.

Source: Systems Applications, Inc. 1980.

TABLE E-111. END-USE DISTRIBUTION - 1978 MIXED XYLENE AND XYLENE ISOMERS

	Usage	
	10^6 lb/yr	%
Mixed xylene as BTX (not isolated)	69,418	
Gasoline	69,418	100.0
Isolated mixed xylene	8,555	
p-xylene isomer	4,107	48.0
o-xylene isomer	1,046	12.2
m-xylene isomer	88	1.0
Ethylene benzene	220	2.6
Gasoline backblending	2,158	25.2
Paint and coating solvent	496	5.8
Adhesives solvent	77	0.9
Chemical manufacturing solvent	77	0.9
Agricultural solvent	66	0.8
Other miscellaneous solvents	55	0.7
Net export	165	1.9
o-xylene	1,046	
Phthalic anhydride	670	64.1
Gasoline backblending	21	2.0
Exports	355	33.9
p-xylene	4,107	
Terephthalic acid	1,430	34.8
Dimethyl terephthalate	2,040	49.7
Net exports	620	15.1
Gasoline backblending	17	0.4
m-xylene	88	
Isophthalic acid	98[a]	100.0

[a]Difference between production and use supplied by imports.

Source: Systems Applications, Inc., 1980.

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TABLE E-112. XYLENE ISOMER END-USERS

Company	Location	Production capacity, 10^6 lb/yr	o-Xylene used, 10^6 lb/yr	Geographic coordinates, Latitude/longitude
Phthalic Anhydride Producers (o-xylene)				
Allied	El Segundo, CA	36	26	33 56 30/118 26 35
BASF Wyandotte	Kearny, NJ	150	107	40 45 53/74 09 03
Exxon	Baton Rouge, LA	130	93	30 09 10/90 54 20
Koppers	Cicero, IL	235	168	41 48 44/87 45 04
Monsanto	Texas City, TX	150	107	29 22 45/94 33 30
Hooker	Arecibo, PR	87	62	Not in project scope
Chevron	Richmond, CA	50	36	37 56 12/122 20 48
Stepan	Millsdale, IL	100	71	41 26 03/88 09 48
Total		938	670	
Isophthalic Acid Producer (m-xylene)				
Amoco	Joliet, IL	240	98	41 26 48/88 10 41

(continued)

TABLE E-112 (continued)

Company	Location	Production capacity, 10^6 lb/yr	o-Xylene used, 10^6 lb/yr	Geographic coordinates, Latitude/longitude
Dimethylterephthalic Acid Producers (o-xylene)				
DuPont	Old Hickory, TN	550	273	36 16 24/86 34 12
	Wilmington, NC	1250	622	34 10 00/77 56 06
Eastman Kodak	Columbia, SC	500	249	33 59 50/81 04 17
	Kingsport, TN	500	249	36 31 41/82 12 22
Hercofina	Wilmington, NC	1300	647	34 19 27/77 46 56
Total		4100	2040	
Terephthalic Acid Producers (p-xylene)				
Amoco	Cooper River, SC	1000	441	32 45 57/79 58 28
	Decatur, AL	2000	883	34 36 12/86 58 42
Hercofina	Wilmington, NC	240	106	34 19 27/77 46 56
Total		3240	1430	

Source: Systems Applications, Inc., 1980.

TABLE E-113. 1978 NATIONWIDE EMISSIONS OF XYLENE ISOMERS

	Nationwide emissions, lb/yr
p-xylene	
Mixed xylene production	1,610,076
Mixed xylene solvent use	114,395,000
Ethyl benzene production	7,348
p-Xylene production	6,447,990
Terephthalic acid production	469,200
Dimethylterephthalate production	3,889,600
Gasoline marketing - evaporation	2,138,500
Gasoline automobile - evaporation	1,967,100
Gasoline automobile - exhaust	108,345,600
Total	239,270,414
o-xylene	
Mixed xylene production	1,976,440
Mixed xylene solvent use	140,425,000
Ethyl benzene production	9,020
o-Xylene production	2,667,300
Phthalic anhydride	134,000
Gasoline marketing - evaporation	2,138,500
Gasoline automobile - evaporation	1,967,100
Gasoline automobile - exhaust	119,180,000
Total	268,497,360
m-xylene	
Mixed xylene production	3,706,331
Mixed xylene solvent use	244,545,000
Ethyl benzene production	15,708
m-Xylene production	176,000
Isophthalic acid	98,000
Gasoline marketing - evaporation	5,193,400
Gasoline automobile - evaporation	4,777,400
Gasoline automobile - exhaust	195,022,100
Total	453,533,939

Source: Systems Applications, Inc., 1980.

TABLE E-114. XYLENE ISOMER EMISSIONS FROM XYLENE ISOMER PRODUCERS

Company	Location	Emissions, lb/yr			Total emissions	
		Process	Storage	Fugitive	lb/yr	g/s
o-xylene Producers						
ARCO	Houston, TX	382,470	14,640	69,540	466,650	6.72
Corco	Ponce, PR	319,770	12,240	58,140	390,150	5.62
Exxon	Baytown, TX	363,660	13,920	66,120	443,700	6.39
Monsanto	Chocolate Bayou, TX	54,340	2,080	9,880	66,300	0.95
Phillips	Guayama, PR	237,170	9,040	42,940	289,150	4.15
Shell	Deer Park, TX	300,960	11,520	54,720	367,200	5.28
Sun	Corpus Christi, TX	292,600	11,200	53,200	357,000	5.14
Tenneco	Chalmette, LA	236,170	9,040	42,940	288,150	4.15
Total		2,187,140	83,680	397,480	2,668,300	
m-xylene Producer						
Amoco	Texas City, TX	139,040	10,560	26,400	176,000	2.53
p-xylene Producers						
Amoco	Decatur, AL	1,085,280	180,880	228,480	1,494,640	21.52
	Texas City, TX	751,260	125,210	158,160	1,034,630	14.89
ARCO	Houston, TX	300,960	50,160	63,360	414,480	5.97
Chevron	Pascagoula, MS	275,880	45,980	58,080	379,940	5.47
St. Croix	St. Croix, VI	501,600	83,600	105,600	690,800	9.94
Exxon	Baytown, TX	351,120	58,520	73,920	483,560	6.96
Hercor	Penuelas, PR	501,600	83,600	105,600	690,800	9.94
Phillips	Guayama, PR	392,160	65,360	82,560	540,080	7.78
Shell	Deer Park, TX	91,200	15,200	19,200	125,600	1.81
Sun	Corpus Christi, TX	326,040	54,340	68,640	449,020	6.46
Tenneco	Chalmette, LA	104,880	17,480	22,080	144,440	2.08
Total		4,681,980	780,330	985,680	6,447,990	

Source: Systems Applications, Inc., 1980.

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TABLE E-115. MIXED XYLENE EMISSIONS FROM OTHER MIXED XYLENE PRODUCERS

Company	Location	Emissions, lb/yr			Total emissions	
		Process	Storage	Fugitive	lb/yr	g/s
Pyrolysis-Gasoline						
ARCO	Channelview, TX	17,290	74,100	7,410	98,800	1.42
Commonwealth	Penuelas, PR	8,470	36,300	3,630	48,400	0.70
Dow	Freeport, TX	5,320	22,800	2,280	30,400	0.44
Exxon	Baton Rouge, LA	3,850	16,500	1,650	22,000	0.32
Gulf	Cedar Bayou, TX	2,590	11,100	1,110	14,800	0.21
Mobile	Beaumont, TX	1,890	8,100	810	10,800	0.16
Monsanto	Texas City, TX	5,880	25,200	2,520	33,600	0.48
Shell	Deer Park, TX	2,940	12,600	1,260	16,800	0.24
Union Carbide	Taft, LA	9,590	41,100	4,110	54,800	0.79
Total		57,820	247,800	24,780	330,400	
Coal-Derived						
Ashland	Catlettsburg, KY	6,500	7,800	1,950	16,250	0.23
	N. Tonawanda, NY	3,500	4,200	1,050	8,750	0.13
U.S. Steel	Clairton, PA	6,500	7,800	1,950	16,250	0.23
Total		16,500	19,800	4,950	41,250	
Toluene Disproportionation						
ARCO	Houston, TX	4,850	9,700	4,850	19,400	0.29
Sun	Marcus Hook, PA	5,050	10,100	5,050	20,200	0.30
Total		9,900	19,800	9,900	39,600	

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TABLE E-116. MIXED XYLENE EMISSIONS FROM CATALYTIC REFORMATE (ISOLATED MIXED XYLENES) PRODUCTION

Company	Location	Emissions, lb/yr			Total emissions	
		Process	Storage	Fugitive	lb/yr	g/s
Amerada Hess	St. Croix, VI	20,070	40,140	20,070	80,280	1.16
American Petrofina	Big Springs, TX	9,180	18,360	9,180	36,720	0.53
	Beaumont, TX	2,160	4,320	2,160	8,640	0.12
Ashland Oil	Catlettsburg, KY	4,290	8,580	4,290	17,160	0.25
	N. Tonawanda, NY	2,010	4,020	2,010	8,040	0.12
ARCO	Houston, TX	11,340	22,680	11,340	45,360	0.65
Charter Oil	Houston, TX	1,590	3,180	1,590	6,360	0.09
Cities Service	Lake Charles, LA	7,170	14,340	7,170	28,680	0.41
Costal States	Corpus Christi, TX	2,400	4,800	2,400	9,600	0.14
Commonwealth	Penuelas, PR	15,060	30,120	15,060	60,240	0.87
Crown	Pasadena, TX	2,010	4,020	2,010	8,040	0.12
Exxon	Baytown, TX	17,910	35,820	17,910	71,640	1.02
Gulf	Alliance, LA	8,610	17,220	8,610	34,440	0.50
Kerr-McGee	Corpus Christi, TX	6,150	12,300	6,150	24,600	0.35
Marathon	Texas City, TX	1,590	3,180	1,590	6,360	0.09

(continued)

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TABLE E-116 (continued)

Company	Location	Emissions, lb/yr			Total emissions	
		Process	Storage	Fugitive	lb/yr	g/s
Monsanto	Texas City, TX	1,410	2,820	1,410	5,640	0.08
Phillips	Guayama, PR	14,310	28,620	14,310	57,240	0.82
Quitana-Howell	Corpus Christi, TX	1,830	3,660	1,830	7,320	0.11
Shell	Deer Park, TX	10,770	21,540	10,770	43,080	0.62
Chevron	Pascagoula, MS Richmond, CA	9,300 8,610	18,600 17,220	9,300 8,610	37,200 34,440	0.54 0.50
Amoco	Texas City, TX Whiting, IN	35,130 25,800	70,260 51,600	35,130 25,800	140,520 103,200	2.02 1.49
Sun	Corpus Christi, TX Marcus Hook, PA Toledo, OH	3,420 2,850 7,170	6,840 5,700 14,340	3,420 2,850 7,170	13,680 11,400 28,680	0.20 0.16 0.41
Tenneco	Chalmette, LA	5,700	11,400	5,700	22,800	0.33
Union Oil	Chicago, IL	1,440	2,880	1,440	5,760	0.08
Union Pacific	Corpus Christi, TX	450	900	450	1,800	0.03
Total		239,730	479,460	239,730	958,920	

Source: Systems Applications, Inc., 1980.

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TABLE E-117. XYLENE ISOMER EMISSIONS FROM USERS

Company	Location	Emissions, lb/yr			Total emissions	
		Process	Storage	Fugitive	lb/yr	g/s
Phthalic Anhydride Producers (o-xylene)						
Allied	El Segundo, CA	3,640	520	1,040	5,200	0.07
BASF Wyandotte	Kearny, NJ	14,980	2,140	4,280	21,400	0.31
Exxon	Baton Rouge, LA	13,020	1,860	3,720	18,600	0.27
Koppers	Ciecero, IL	23,520	3,360	6,720	33,600	0.48
Monsanto	Texas City, TX	14,980	2,140	4,280	21,400	0.31
Hooker	Arecibo, PR	8,680	1,240	2,480	12,400	0.18
Chevron	Richmond, CA	5,040	720	1,440	7,200	0.10
Stepan	Millsdale, IL	9,940	1,420	2,840	14,200	0.20
Total		93,800	13,400	26,800	134,000	
Isophthalic Acid Producer (m-xylene)						
Amoco	Joliet, IL	83,000	4,900	9,800	98,000	1.41
Dimethylterephthalate Producers (p-xylene)						
DuPont	Old Hickory, TN	35,490	8,190	19,110	62,790	0.90
	Wilmington, NC	87,360	18,660	43,540	149,560	2.15
Eastman Kodak	Columbia, SC	32,370	7,470	17,430	57,270	0.82
	Kingsport, TN	32,370	7,470	17,430	57,270	0.82
Hercofina	Wilmington, NC	84,110	19,410	45,290	148,810	2.14
Total		271,700	61,200	142,800	475,700	
Terephthalic Acid Producers (p-xylene)						
Amoco	Cooper River, SC	1,120,140	48,510	30,870	1,199,520	17.27
	Decatur, AL	2,242,820	97,130	61,810	2,401,760	34.58
Hercofina	Wilmington, NC	269,240	11,660	7,420	288,320	4.15
Total		3,632,200	157,300	100,100	3,889,600	

Source: Systems Applications, Inc., 1982.

TABLE E-118. XYLENE ISOMER EMISSIONS FROM MIXED XYLENE SOLVENT USES

	Total mixed xylene emissions, 10^6 lb/yr	p-xylene emissions, 10^6 lb/yr	o-xylene emissions, 10^6 lb/yr	m-xylene emissions, 10^6 lb/yr
Paints and coatings	422	70.474	86.510	150.654
Adhesive, rubber	77	12.859	15.785	27.489
Chemical, automotive	65	10.855	13.325	23.205
Agricultural pesticides	66	11.022	13.530	23.562
Household products, printing inks	55	9.185	11.275	19.635
Total	685	114.395	140.425	244.545

Source: Systems Applications, Inc., 1980.

TABLE E-119. XYLENE ISOMER EMISSIONS FROM GASOLINE MARKETING

Region	Number of sites	o-xylene emissions, lb/yr	m-xylene emissions, lb/yr	p-xylene emissions, lb/yr
New England	11,105	104,831	254,638	104,831
Middle Atlantic	28,383	267,935	650,822	267,935
East North Central	42,270	399,029	969,251	399,029
West North Central	23,304	219,990	534,361	219,990
South Atlantic	37,286	351,980	854,968	351,980
East South Central	16,313	153,995	374,057	153,995
West South Central	28,336	267,492	649,744	267,492
Mountain	12,815	120,974	293,848	120,974
Pacific	26,647	251,548	611,016	251,548
Total	226,459	2,137,774	5,192,705	2,137,774

Source: Systems Applications, Inc., 1982.
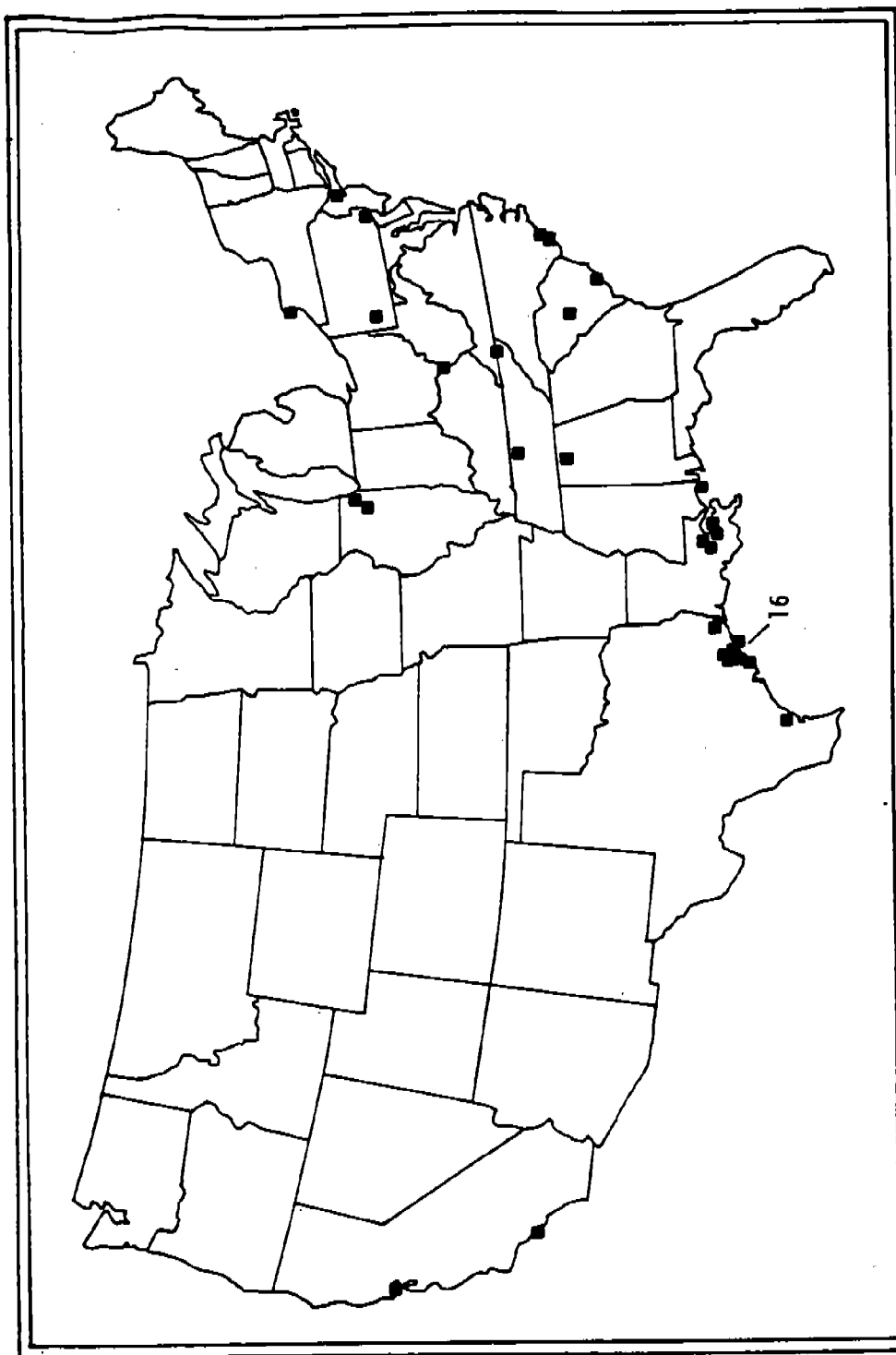
NOTE: NUMERALS DENOTE NUMBER OF PLANTS.

Figure E-8. Specific point sources of o,m,p-xylene emissions.

Source: Systems Applications, Inc., 1980.

Sampling and Analytical Methods

1. NIOSH Method 1501
   a. Solid Sorbent Tube (coconut shell charcoal, 100 mg/50 mg).
   b. Gas chromatography.
   c. Flame ionization detector.

   Detection limit:
   0.2 ppm for 10-liter sample

   Possible interferences:
   Alkanes less than C_{10} along with volatile organic solvents (e.g., alcohols, keytones, ethers, and halogenated hydrocarbons).

2. Method B (Appendix A): C_2-C_{18} hydrocarbons and other nonpolar organics with a boiling point of 100° to 175°C.
   a. Whole air collection in canister.
   b. Cryogenic concentration.
   c. Gas chromatography/flame ionization detection (gas chromatography/photoionization detection may also be used).

   Detection limit:
   0.1 ppb per 100-ml sample

   Possible interferences:
   Reactive compounds are not readily analyzed. Storage times greater than a week are not recommended.

3. Method C (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with a boiling point of 60° to 200°C.
   a. Adsorption of Tenax (XAD-2 with solvent extraction may be used).
   b. Thermal desorption.
   c. Gas chromatography/mass spectrometry analysis (gas chromatography/photoionization detection may also be used).

   Detection limit:
   1 to 200 ppt for a 20-liter sample

   Possible interferences:
   Blank levels usually limit sensitivity artifacts due to reactive components (O_3, NO_x). Sample can be analyzed only once.

4. Method D (Appendix A): C_6-C_{12} hydrocarbons and other nonpolar organics with a boiling point of 60° to 200°C.
   a. Adsorption of Tenax (XAD-2 with solvent extraction may be used).
   b. Thermal desorption into canisters.

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c. Gas chromatography/flame ionization detection, or gas chromatography/mass spectrometry analysis (gas chromatography/photoionization detection may also be used).

Detection limit:
    0.01 to 1 ppb for a 20-liter sample

Possible interferences:
    Blanks and artifact problems in Method C, above.

Permissible Exposure Limits

	OSHA	ACGIH	NIOSH
TWA	100 ppm (435 mg/m³)	100 ppm (435 mg/m³)	100 ppm
Ceiling			200 ppm (10 min)
STEL		150 ppm (655 mg/m³)	

Human Toxicity

Acute Toxicity:
    Human eye and skin irritation can start at 200 ppm. Moderate irritant through intraperitoneal, subcutaneous, and inhalation means. Low toxicity orally. Very little dermal toxicity. At high concentrations, xylene vapor may cause severe breathing difficulties, which may be delayed in onset. At high concentration, may also cause dizziness, staggering, drowsiness, and unconsciousness. In addition, breathing high concentrations may cause lack of appetite, nausea, vomiting, abdominal pain, and reversible damage to kidneys and liver.

Chronic Toxicity:
    Repeated exposure of the eyes to high concentrations of xylene vapor may cause reversible eye damage.

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APPENDIX F

GUIDANCE FOR THE CHOICE OF MONITORING FREQUENCY
TO BE USED IN ESTIMATING ANNUAL AVERAGE CONCENTRATIONS
OF NONCRITERIA AIR POLLUTANTS

Prepared by

Systems Applications, Inc.
101 Lucas Valley Road
San Rafael, California 94903

Monitoring Section
Monitoring and Data Analysis Division
U.S. Environmental Protection Agency
Research Triangle Park, North Carolina 27711

April 1985

ACKNOWLEDGMENT

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ABSTRACT

The reliability of the estimated annual average concentration of a
noncriteria air pollutant is considered. The increase in precision
resulting from more frequent monitoring is illustrated, and guidance on
the selection of a monitoring frequency to achieve a desired precision is
provided.

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DISCLAIMER

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CONTENTS

INTRODUCTION

There are at present no national ambient air quality standards for a number of air pollutants considered to be of possible harm to public health. Planning is in progress, and some programs are already underway, by national, state, and local agencies, to monitor these so-called noncriteria air pollutants. The monitoring data will be used for many purposes, e.g., to estimate air quality trends, population exposure, or the influence of emissions.

In allocating funds for these programs, it is important to determine where and how often the pollutants must be monitored to achieve stated objectives. In this report we restrict attention to the sampling frequency required to reliably estimate annual average concentrations. Other monitoring objectives, as well as the costs and health benefits of various monitoring alternatives, although very important, are not discussed here. In particular, the monitoring of high concentrations of short duration will be addressed in a future report.

Our purpose is thus to quantify and illustrate the effect of sampling frequency on the precision of the sample annual average concentration of a noncriteria air pollutant. It should be noted that even within this narrowly defined context we have had to set aside from our discussion certain important aspects of the design or evalution of a monitoring program such as measurement error, minimum detection limits, quality assurance, or the determination of just how much precision is needed. Nevertheless the results and examples presented should provide some useful information on the design and evaluation of monitoring programs.

It should also be noted that the determination of monitoring objectives, the development and understanding of alternative monitoring methods, and the design of programs to meet these objectives are evolving in concert through ongoing activities. Specifically, several state and local agencies are currently monitoring noncriteria air pollutants, and the U.S. Environmental Protection Agency has a pilot phase of the Toxic Air Monitoring System (TAMS) underway.

MONITORING PROGRAMS

The Toxic Air Monitoring System (TAMS)

The U.S. Environmental Protection Agency (EPA) is currently developing a Toxic Air Monitoring System (TAMS), a network of stations to monitor up to 60 noncriteria air pollutants. One important goal of the TAMS is to enable researchers to assess long-term exposures to toxic air pollutants, hence our emphasis on the estimation of annual average concentrations.

An important limitation of the monitoring program is that precipitation interferes with the measurement of certain volatile organic compounds (VOC's) collected on Tenax adsorbent material. Lumpkin and Bond (1984) state that samples of this type taken during precipitation should not be used, however other monitoring methods less vulnerable to precipitation are under study.

Another important aspect of the monitoring program is that samplers must be operated at different flow rates and for different sampling periods to effectively monitor different compounds. For some VOC's the usual 24-hour integrated samples are not possible because the 24-hour air volume would exceed the retention volume (Walling, 1984). Thus, shorter sampling periods, e.g., 12-hour or 6-hour integrated samples, may be required. This adds the dimension of time of day to the design of the monitoring program.

The EPA plans to conduct a pilot monitoring program in a few urban areas (beginning with Boston, Chicago, and Houston) before the national network is established. The current sampling plan for the TAMS pilot network is to monitor at each site (1) certain volatile organic compounds (VOC's) collected on Tenax, (2) formaldehyde, (3) benzo(a)pyrene (BaP), and (4) the trace metals arsenic, cadmium, chromium, and nickel. Twelve-hour or 6-hour integrated samples of VOCs will be taken. Either 12- or 24-hour integrated samples of formaldehyde will be taken, and 24-hour integrated samples of BaP and the metals will be taken using high-volume ("hi-vol") particulate samples. The experience and data gained from the pilot program will enable the EPA to conduct the larger effort with greater efficiency.

Toxic Air Monitoring by State and Local Agencies

In addition to the planned national system for monitoring noncriteria air pollutants, many state and local agencies have or are planning programs to monitor these pollutants. A practical limitation of these programs, shared by national programs, is that only a proportion of the scheduled samples yield valid observations. Planned observations may be missed or

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invalidated because of precipitation or equipment failure, for example. The proportion of valid observations is known as the data capture rate.

ISSUES

A number of issues related to the TAMS are discussed by Thrall, Burton, and Moezzi (1984). These issues include the estimation of diurnal or seasonal components of variation, trade-offs between infrequent monitoring at several sites versus more frequent monitoring at one site, and the precision required of estimated annual concentrations given the uncertainty of our knowledge of the health risks associated with different pollutants.

In addition to the issues arising in national monitoring programs, a state or local agency may face the issue of determining whether the annual average concentration of a noncriteria pollutant is sufficiently high at some particular site to be of concern. If the concentration at which chronic human health effects occur is known, then the agency may wish to monitor the pollutant with sufficient frequency so that reliable comparisons can be made between the estimated annual average concentration and the specified annual mean level of concern. When the concentration at which chronic health effects occur cannot be specified, the agency may nevertheless wish to compare estimated annual averages to levels observed at other sites or during previous years so that sites requiring more intensive investigation can be identified.

Another issue is the monitoring frequency required to produce estimated annual averages of specified reliability. In this case, the agency's concern would be the more general one of obtaining data (i.e., estimated averages) of good quality. The two issues we discuss may be summarized as follows.

Reliability of Comparisons: What frequency of monitoring is required to produce reliable comparisons between the estimated annual average concentration and some specified level?

Reliability of Estimates: What frequency of monitoring is required to produce reliable estimates of the average of ambient concentrations over the entire course of the year, i.e., the average that would be obtained from an uninterrupted data record?

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SOURCES OF INFORMATION

The TAMS network will provide needed information about the level and variability of noncriteria air pollutants. Although profiles of these pollutants have been compiled (see, e.g., Hunt, Faoro, and Duggan, 1984; Koch et al., 1984; and Singh et al., 1977, 1979, 1983), long-term records of ambient concentrations are rare. Our recommendations and examples are based on one of the few such long-term records. The California Air Resources Board (CARB) monitored trichloroethylene, carbon tetrachloride, and chloroform in El Monte from November 1982 through September 1983 and in three other sites in the Los Angeles area from January through September 1983. The data collected by the CARB are discussed by Hunt (1984) and by Thrall, Burton, and Moezzi (1984) and are summarized here in Table 1.

The concentrations reported in Table 1 represent 24-hour integrated samples. The data include 14 instances in which concentrations were below the lower detection limit of the monitoring instrument but were reported as equalling the instrument's lower limit. The data also include some suprisingly high concentrations, notably a 3 ppb concentration of chloroform recorded in downtown Los Angeles on 29 March 1983. These reported concentrations have been confirmed by both EPA and CARB technical staff, that is, the concentrations do not appear to be the result of transcription errors or faulty chemical analysis. For the time being we interpret these concentrations as indicative of occasionally high values at these sites, although the possibility remains that they are the result of either some gross error in the measurement process or some very unusual event.

THE PRECISION RESULTING FROM COMBINATIONS OF
SAMPLING AND POLLUTANT CHARACTERISTICS

The bias and imprecision of estimated annual average concentrations serve as criteria to assess the need for more or less frequent monitoring of VOC's and other noncriteria air pollutants. Within the resources available, it is also important to accurately estimate variances, that is, to get some indication of the geographic variability of annual average concentrations within an urban area, and to obtain reliable estimates of the extremes and standard deviation of concentrations at a site over the course of a year, particularly during the initial operation of a network.

We emphasize, however, that we are restricting attention to the statistical reliability of estimated annual average concentrations, as mentioned in the introduction. That is, there are other important issues beyond the scope of the present discussion, such as the comparative costs of implementing various monitoring strategies, alternative monitoring objectives

TABLE 1. Summary statistics for three volatile organic compounds (VOCs) monitored at four sites in the Los Angeles Area from November 1982 through September 1983 (concentrations are expressed in parts per billion).

Pollutant	Statistic	El Monte	Downtown Los Angeles	Dominquez	Riverside	Combined
Trichloroethylene	Average	0.289	0.565	0.283	0.327	0.331
	Standard Dev.	0.230	0.295	0.158	0.185	0.245
	Coefficient of Var.	0.796	0.522	0.560	0.566	0.739
	Maximum	1.200	1.500	0.680	0.870	1.500
	Minimum	0.020	0.020	0.100	0.020	0.020
	Sample Size	180	42	43	37	302
Carbon Tetrachloride	Average	0.039	0.037	0.041	0.036	0.038
	Standard Dev.	0.009	0.008	0.012	0.007	0.009
	Coefficient of Var.	0.242	0.224	0.297	0.193	0.247
	Maximum	0.073	0.060	0.080	0.060	0.080
	Minimum	0.010	0.010	0.030	0.030	0.010
	Sample Size	179	41	43	36	299
Chloroform	Average	0.062	0.144	0.051	0.061	0.072
	Standard Dev.	0.096	0.454	0.024	0.061	0.187
	Coefficient of Var.	1.542	3.148	0.471	1.007	2.611
	Maximum	1.100	3.000	0.140	0.400	3.000
	Minimum	0.020	0.020	0.020	0.020	0.020
	Sample Size	179	42	42	37	300

(e.g., comparing the influence on air quality of different sources of pollutant emissions, or estimating peak concentrations), or the public health benefits of the information to be gained from monitoring.

The trade-off between precision and sampling frequency is illustrated in Table 2 for sampling frequencies of 1/3, 1/6, 1/12. The table gives 95 percent confidence bounds on the magnitude of the error of the estimated annual average expressed as a percentage of the actual annual average (i.e., the relative difference, expressed as a percentage, between the estimated and actual averages). These bounds have been obtained from a normal distribution that approximates the sampling distribution of the estimated annual average concentration for a data capture rate (percentage of scheduled observations yielding valid data) ranging from 50 to 100 percent, and for a coefficient of variation (the standard deviation divided by the average, thus the relative variation about the average) ranging from 25 to 300 percent.

Table 2 shows, for example, that monitoring carbon tetrachloride at one of the four sites in the Los Angeles area with a 100 percent data capture rate will result in a relative error likely to be no more than 4 percent if 24-hour concentrations (or two consecutive 12-hour concentrations) are monitored once every three days. The bound changes from 4 percent to 9 percent if monitoring is scheduled once every 12 days. At the other end of the scale, monitoring chloroform in downtown Los Angeles with only a 50 percent data capture rate could result in a 69 percent error if monitoring were scheduled every three days, and a 148 percent error if monitoring were scheduled every 12 days.

Note that the table also provides precision bounds for monitoring 12-hour concentrations alternately during the night and day. One can, of course, effectively construct 24-hour observations by sampling during consecutive 12-hour periods. Alternatively, monitoring 24-hour concentrations once every 3, 6, or 12 days corresponds to monitoring 12-hour concentrations once every 36 hours, three days, or six days, respectively.

Similarly, the table can be interpreted for 6-hour samples. Again, 24-hour averages can be formed if four consecutive 6-hour samples are taken at a time. The table then applies to blocks of 4 consecutive samples taken once every 3, 6, or 12 days. More generally, the table applies to sampling schedules that call for monitoring a representative one-third, one-sixth, or one-twelfth of the total number of possible sampling periods.

An important assumption used in the construction of the table is that the probability of data capture is independent of the probability of the occurrence of either high or low concentrations. Entries in the table

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TABLE 2. Ninety-five percent confidence bounds on the magnitude of the error of the annual average concentration estimated from scheduled monitoring of 24-hour concentrations once every three, six, or 12 days, respectively, when the error is expressed as a percentage of the actual annual average concentration.

Data Capture Rate (%)	Sampling Frequency	Coefficient of Variation (%)					
		25[a]	50	75[b]	100	200	300[c]
100	1/3	4	7	11	15	29	44
	1/6	6	11	17	23	46	69
	1/12	9	17	26	34	68	102
90	1/3	4	8	12	16	31	47
	1/6	6	12	18	24	49	73
	1/12	9	18	27	36	72	108
80	1/3	4	9	13	17	34	51
	1/6	7	13	20	26	52	78
	1/12	10	19	29	38	77	115
70	1/3	5	9	14	19	37	56
	1/6	7	14	21	28	56	85
	1/12	10	21	31	41	82	124
60	1/3	5	10	15	21	41	62
	1/6	8	15	23	31	62	92
	1/12	11	22	34	45	89	134
50	1/3	6	11	17	23	46	69
	1/6	9	17	26	34	68	102
	1/12	12	25	37	49	98	148

[a] 25 percent corresponds roughly to the combined CV for carbon tetrachloride in Table 1.

[b] 75 percent corresponds roughly to the combined CV for trichloroethylene in Table 1.

[c] 300 percent corresponds roughly to the combined CV for chloroform in Table 1.

would have to be modified if it were known, for example, that daytime concentrations tended to be higher or lower than nighttime concentrations and that a disproportionate number of, say, nighttime observations would fail to yield valid data.

From the table we see that for a pollutant and site for which the coefficient of variation and data capture rate are known, or can be estimated, precision increases roughly in proportion to the square of the expected number of valid observations. For example, the error bound for samples taken once every 12 days is roughly twice that for samples taken once every three days.

In designing a network consideration must be given to: (1) the expected data capture rate (including loss of samples due to precipitation); (2) the likely coefficients of variation of different pollutants at different sites; and (3) the desired bounds on the percentage error of estimated annual average concentrations. Thrall, Burton, and Moezzi (1984) discuss these and other considerations in their review of the CARB data.

EXAMPLES OF TRADE-OFFS BETWEEN PRECISION
AND SAMPLING FREQUENCY

In choosing a monitoring frequency, one should consider not only the desired level of precision, but also the likely data capture rate (the proportion of scheduled monitoring days that yield valid observations), and the number and types of sources of pollutant emissions that would influence the level and variability of ambient concentrations from day to day. The following examples illustrate this point.

Example 1. Suppose that the annual average concentration of trichloro-ethylene at a new monitoring site is to be compared to the approximately 0.3 ppb recorded at three of the four sites located in the Los Angeles area listed in Table 1. Suppose also that we are willing to assume that the daily ambient concentrations at the new site are not much more variable than those at the Los Angeles sites, i.e., that the coefficient of variation (the standard deviation expressed as a percentage of the annual average) at the new site is 100 percent (the maximum coefficient of variation among the four Los Angeles sites is about 80 percent), and that the likely data capture rate will be 75 percent.

Finally, we want to be confident that the estimated average concentration will fall below 0.3 ppb if the actual value is below 0.3 ppb, and, conversely, that the estimate will fall above 0.3 ppb if the actual average is above 0.3 ppb. Of course, if the actual average concentration equals

0.3 ppb or is very close to this level, the estimate may easily fall above or below the 0.3 ppb level. So, to be more precise, we may require sufficiently frequent monitoring such that, say, with 90 percent probability, the estimate will fall on the same side of the 0.3 ppb level as the actual average, provided that the magnitude of the relative difference between the specified 0.3 ppb level and the actual annual average concentration at the site is at least 10 percent.[*] Under these circumstances the required frequency of scheduled monitoring is about once every three days. The derivation of the required monitoring frequency will be explained shortly.

Example 2. Suppose now that we plan to compare the annual average concentration of chloroform to be obtained at the new site with the approximately 0.06 ppb obtained at the same three Los Angeles sites as in Example 1. Suppose, again, that the data capture rate is 75 percent, and that we want to be 90 percent confident of a correct comparison, provided that the magnitude of the relative difference between the specified 0.06 ppb level and the actual average concentration is at least 10 percent. The required sampling frequency now depends on whether the relative variability, i.e., the coefficient of variation, of daily ambient concentrations at the new site resembles that of Riverside or that of downtown Los Angeles. A site resembling Riverside would have a coefficient of variation of about 100 percent, and the required sampling frequency would again be about once every three days. A site resembling downtown Los Angeles would have a coefficient of variation of about 300 percent, and everyday sampling would be required.

The required frequency can be formulated as follows. If we let f denote the frequency of scheduled monitoring, then f^{-1} is the period between scheduled samples, so that monitoring is scheduled "once every f^{-1} days" (or, more generally, once every f^{-1} time intervals). In Examples 1 and 2, f^{-1} was obtained using the following formula (derived in the appendix):

$$f^{-1} = p \cdot \left(1 + \frac{N \cdot r_L^2}{CV^2 \cdot z^2} \right) \qquad (1)$$

where

p = the proportion of scheduled monitoring days that yield valid observations, also known as the data capture rate; in our exampes $p = 0.75$;

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[*] The "relative difference" between two numbers, x and y, is (x - y)/y.

N = the total number of time intervals in a year, e.g., N = 365 in our examples, corresponding to the number of 24-hour intervals in a year;

r_L = a lower limit on the magnitude of the relative difference between the specified level and the new site's actual annual average concentration; r = 0.1 in our examples; corresponding to our objective of identifying differences as great or greater than 10 percent;

CV = the coefficient of variation (the ratio of the standard deviation divided by the average) at the new site, e.g., 1.0 to 3.0 in our examples;

z = the percentile of the standard normal distribution, corresponding to the level of confidence desired for a correct comparison; in our examples z = 1.282, corresponding to the desired 90 percent level of confidence; in general, setting z equal to the (1- α)th quantile produces a (1 - α) level of confidence, 90 or 95 percent being typical choices in statistical applications.

Generally, Equation 1 should be regarded as providing an initial approximation to the required monitoring frequency. If the number of valid observations per year (f·p·N) is less than 20, then it is advisable to override Equation 1 with the recommendation of Hunt, Faoro, and Duggan (1984) that at least five valid observations per quarter be obtained. Similarly, it is wise to avoid monitoring exclusively on one day of the week, even if such a schedule is obtained from Equation 1, because pollutant levels may differ substantially on different days of the week. Finally, a once-per-six-day monitoring schedule is common among many agencies, and it may be practically important to coordinate the new schedule with existing schedules. Since Equation 1 approximates the minimum amount of monitoring needed to meet specified criteria, any adjustments to the derived sampling frequency should generally be in the direction of providing more frequent monitoring. The next examples illustrate these suggestions.

Example 3. Suppose that the annual average concentration of carbon tetrachloride at the new monitoring site is to be compared to the approximate 0.04 ppb obtained at the four sites in the Los Angeles area listed in Table 1. Suppose, again, that the expected data capture rate is 75 percent (p = 0.75), and that we want to be 90 percent confident of a correct comparison (z = 1.282, the 90th percentile of the standard normal distribution) if the magnitude of the relative difference between the specified 0.04 ppb level and the new site's actual average concentration is at least

10 percent ($r_L = 0.1$). Finally, let us assume that the coefficient of variation for the new site is only 25 percent (CV = 0.25), which is the approximate value at the Los Angeles sites.

Due to the low coefficient of variation, Equation 1 yields an approximate once-per-34-days sampling schedule ($f^{-1} \doteq 34$), i.e., about 11 scheduled monitoring days per year, which, using the 75 percent data capture rate, can be expected to yield about eight valid observations per year ($f \cdot p \cdot N \doteq 8$). Since this is less than the recommended 20 valid observations per year, we would adopt the suggestion of Hunt, Faoro, and Duggan (1984) that at least five valid observations per quarter be obtained. Based on the 75 percent data capture rate, we might therefore schedule monitoring once every 12 days. (A straightforward calculation yields a sampling schedule of once every 13.7 days; monitoring every 12 days thus allows for a data capture rate in one or more quarters that is somewhat less than 75 percent.)

When we have no specific concentration to which the calculated annual average is to be compared, we may simply require that the average obtained from intermittent monitoring be close to the average of ambient concentrations over the entire course of the year.

One way to express this requirement is that the relative difference between the calculated and underlying annual averages should be, say, less than 10 percent with at least 90 percent probability. Equation 2 (derived in the appendix) provides a formula for calculating the sampling period, f^{-1}, meeting these requirements:

$$f^{-1} = p \cdot \left(1 + \frac{N \cdot r_U^2}{CV^2 \cdot z_2^2} \right) \qquad (2)$$

where r_U is the desired upper limit (e.g., 0.1) on the magnitude of the relative difference, z_2 is the percentile of the standard normal distribution corresponding to the desired confidence level,* and N, p, and CV are as given under Equation 1. Again, Equations 1 and 2 merely provide an initial approximation to the required monitoring frequency (see the remarks following Equation 1).

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* To achieve the confidence level $1 - \alpha$, z_2 should be the $1 - (\alpha/2)$ quantile of the standard normal distribution, e.g., z_2 should be the 95th percentile (1.645) to achieve 90 percent confidence.

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Example 4. Suppose that a state or local agency plans to monitor 24-hour concentrations of carbon tetrachloride sufficiently often so that the relative difference between the estimated and actual annual average concentrations will be no more than 10 percent with 90 percent probability (r_u = 0.1, z_2 = 1.645). The coefficient of variation is assumed to be 25 percent (CV = 0.25), consistent with the data from Table 1, and the data capture rate is assumed to be 75 percent (p = 0.75). Since there are 365 24-hour intervals in the year (N = 365), Equation 2 yields an approximate sampling schedule of once every 17 days ($f^{-1} \doteq 17$). However, since the expected number of valid observations is less than 20 (f·p·N is approximately 16), a schedule of once every 12 days would be more appropriate, consistent with the remarks in example 3.

Example 5. Suppose that the situtation is as described in example 4, except that the measurement method is based on 12-hour samples rather than 24-hour samples. Application of the formula for the required sampling frequency now indicates monitoring one out of every seventeen 12-hour intervals. This could be achieved in a number of ways, e.g., monitoring for 12 hours every 8 1/2 days (thus alternating between nighttime and daytime monitoring) or monitoring during two consecutive 12-hour intervals every 17 days. There may be some statistical advantage to one scheme over the other, depending on the pattern of daytime and nighttime concentrations. Also, in order to match other monitoring schedules, it may be more convenient to take alternate nighttime and daytime samples once every six days, or to take two consecutive samples once every twelve days. In any case, if the annual average is to be estimated as the simple arithmetic average of all valid 12-hour samples collected during the year, it is important to obtain about the same number of nighttime and daytime samples. to avoid biasing the estimated annual average.

Example 6. Again, let us suppose that the situation is as described in example 4, this time with 6-hour samples. Equation 2 now indicates monitoring one out of every seventeen 6-hour intervals. This might be accomplished most conveniently by monitoring four consecutive 6-hour intervals once every 17 days. This frequency might be increased to monitoring four consecutive 6-hour intervals once every 12 days to better coincide with other monitoring schedules. Other sampling designs are possible, but if the annual average is to be estimated as the simple arithmetic average of all valid 6-hour samples collected during the year, it is important to obtain approximately the same number of valid observations for each 6-hour interval of the day.

SUMMARY

The development of a program to monitor specified noncriteria air pollutants is a large undertaking with many potential objectives, constraints, and unknowns. This guideline focuses on the monitoring frequency needed to reduce to a specified level the effect of sampling error on the estimated annual average concentration of a pollutant at one monitoring station. "Sampling error" here refers to the fact that the annual average must be estimated from a sample of say, days in the year, since practical constraints limit how often monitoring can be scheduled. In principle the problem of sampling error may be eliminated by monitoring every day or, more generally, during every possible time interval (practically, however, missing or invalid observations can and do occur in this case as well). Thus the guideline addresses one aspect, solvable at least in principle, of a larger and more difficult problem.

Within the sampling error context, a formula is derived in the appendix for the probable error in the estimated annual average as a function of monitoring frequency, data capture rate, and the relative variation of pollutant concentrations over the course of the year. The formula is illustrated in Table 2 and the concluding examples show how related formulas can be used to determine the monitoring frequency needed to limit the probable error to a prescribed magnitude. In some cases where the relative variation in pollutant concentrations is low, the derived infrequent monitoring is overridden by a longstanding EPA recommendation that at least 5 valid observations per quarter be obtained.

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Appendix

DERIVATION OF THE RELATIONSHIP BETWEEN SAMPLING FREQUENCY AND THE PRECISION OF THE ESTIMATED ANNUAL AVERAGE CONCENTRATION

We would like to know the annual average concentration, μ of a pollutant based on a complete set of N measurements. The number of possible observations to be obtained from the schedule of intermittent monitoring is some fraction (f) of N, and only a proportion, p (the so-called "data capture rate") of the scheduled monitoring intervals will produce valid observations. That is, environmental conditions may prohibit scheduled monitoring in some instances; in other cases some mishap in the data collection process may invalidate observations or cause them to be missed. So from a total of N possible measurements we obtain only pfN valid observations, which we regard as a random sample from a finite population.

Letting $\hat{\mu}$ denote the sample average concentration, the expected value and variance of $\hat{\mu}$ are

$$E\hat{\mu} = \mu$$

$$Var\ \hat{\mu} = \frac{1 - fp}{fp} \frac{\sigma^2}{N}$$

where σ^2 is the population variance of the N measurements. Moreoever, if the number of valid and missing (or invalid) measurements is large, i.e., if both pfN and N - pfN are large, and if there are relatively few exteme concentrations, then the sampling distribution of $\hat{\mu}$ is approximately normal. (The conditions for asymptotic normality are formulated more precisely by Cochran, 1963, who cites Hajek, 1960.)

The approximate normality of $\hat{\mu}$ may be conveniently expressed as the approximate normality of the relative error of $\hat{\mu}$:

$$\frac{\hat{\mu} - \mu}{\mu} \sim N(0, \tau_N^2)$$

where

$$\tau_N^2 = \frac{1 - fp}{fp} \frac{CV^2}{N}$$

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Thrall, A. D., C. S. Burton, and M. M. Moezzi. 1984. "Consideration of the Choice of Sampling Frequency to be Used in the Monitoring of Noncriteria Air Pollutants." Systems Applications, Inc., San Rafael, California (SYSAPP-84/212).

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$$CV = \frac{\sigma}{\mu} \text{ is the coefficient variation.}$$

We can use these results to obtain approximate answers to the following two problems.

Problem 1. How frequently should monitoring be scheduled in order to limit the probability of an erroneous comparison of $\hat{\mu}$ to a specified concentration μ_0, i.e., of obtaining $\hat{\mu} > \mu_0$ when $\mu < \mu_0$ or vice versa?

Problem 2. How frequently should monitoring be scheduled to limit the relative error of $\hat{\mu}$ to a prescribed level?

We formulate problem 1 as follows. Since the chance of an erroneous comparison is large if μ is close to μ_0, we suppose that the magnitude of the relative difference between μ_0 and μ is not less than some prescribed lower bound, r_L:

$$\left| \frac{\mu_0 - \mu}{\mu} \right| > r_L.$$

We want the probability of an erroneous comparison to be no more than some prescibed value, say α. Thus, if $\mu > \mu_0$, we require that

$$\alpha > Pr(\hat{\mu} < \mu_0)$$

$$> Pr\left(\frac{\hat{\mu} - \mu}{\mu} < \frac{\mu_0 - \mu}{\mu} \right) \quad .$$

Since the magnitude of the relative difference between μ_0 and μ may be as small as r_L, this implies

$$\alpha > Pr\left(\frac{\hat{\mu} - \mu}{\mu} < - r_L \right)$$
$$= \Phi(- r_L / \tau_N)$$

where Φ is the standard normal cumulative distibution function.

Or, if $\mu < \mu_0$, we require that

$$\alpha > Pr(\hat{\mu} > \mu_0)$$

$$= Pr\left(\frac{\hat{\mu} - \mu}{\mu} > \frac{\mu_0 - \mu}{\mu} \right)$$

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This implies that

$$\alpha \geq \Pr \frac{\hat{\mu} - \mu}{\mu} > r_L$$

$$\doteq 1 - \Phi(r_L/\tau_N)$$

$$= \Phi(- r_L/\tau_N) \text{ from the symmetry of the normal distribution.}$$

Thus, in either case, we require that

$$\alpha \geq \Phi(-r_L/\tau_N) \ ,$$

or

$$1 - \alpha \leq \Phi(r_L/\tau_N) \ ,$$

so that

$$\tau_N^2 \ < \ r_L^2/Z_{1-\alpha}^2 \ ,$$

and hence,

$$\frac{1}{T} < p \left(1 + \frac{N \cdot r_L^2}{CV^2 \cdot Z_{1-\alpha}^2} \right) \ . \tag{1}$$

Here $Z_{1-\alpha}$ denotes the $(1 - \alpha)$th quantile of the standard normal distribution.

Problem 2 can be treated similarly. We want the magnitude of the relative error of $\hat{\mu}$ to be no more than some upper bound, say r_U, with a high probability, say $1 - \alpha$. We thus have

$$1 - \alpha \leq \Pr \left(- r_U \leq \frac{\hat{\mu} - \mu}{\mu} \leq r_U \right)$$

$$= \Phi(r_U/\tau_N) - \Phi(-r_U/\tau_N)$$

$$= 2\Phi(r_U/\tau_N) - 1 \ .$$

Thus

$$1 - \alpha/2 \leq \Phi(r_U/\tau_N) \ .$$

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or

$$Z_{1-\alpha/2} < r_U/\tau_N \, ,$$

so that

$$\tau_N^2 < r_U^2 / Z_{1-\alpha/2}^2 \, ,$$

and hence

$$\frac{1}{f} < p\left(1 + \frac{N \cdot r_U^2}{CV^2 \cdot Z_{1-\alpha/2}^2}\right) \, . \tag{2}$$

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